

Supporting Information
for
Theoretical Study on the Adhesion Interaction between Epoxy Resin
Including Curing Agent and Plated Gold Surface

Yuta Tsuji,¹ Taiki Baba,¹ Naoaki Tsurumi,^{1,2} Hiroyuki Murata,¹ Noriyuki Masago,² Kazunari Yoshizawa^{1*}

1. Institute for Materials Chemistry and Engineering and IRCCS, Kyushu University,
744 Motooka, Nishi-ku, Fukuoka 819-0395, Japan
2. Research and Development Center, ROHM Co., Ltd., 21 Saiin Mizonaki-cho, Ukyo-ku, Kyoto 615-8585, Japan

*To whom correspondence should be addressed.

E-mail: kazunari@ms.ifoc.kyushu-u.ac.jp

Table of Contents

1. Bulk and surface structures of gold	S2
2. 6th-order polynomials used to fit E_{DFT} and $E_{\text{dispersion}}$	S3
3. Change in surface charge with increasing CN coverage	S4
4. Effects of surrounding CN groups on a hydrogen bonding	S5
5. Coordinates of the optimized structures	S7

1. Bulk and surface structures of gold

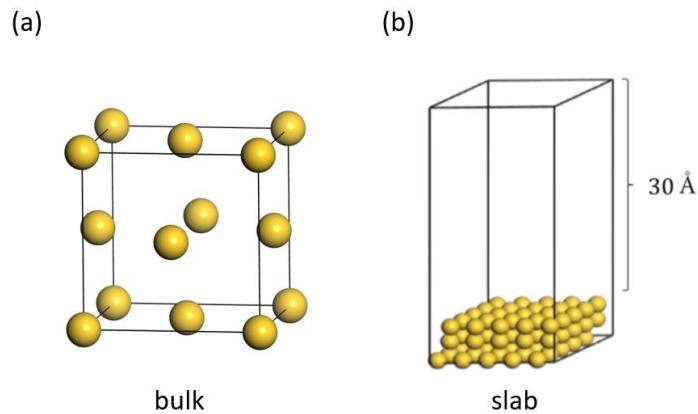


Figure S1. (a) Optimized conventional cell structure of fcc gold and (b) the structure of the (111) surface slab model constructed using this unit cell.

2. 6th-order polynomials used to fit E_{DFT} and $E_{\text{dispersion}}$

With the curing agent

	approximate polynomial	derivative
E_{DFT}	$y = 0.0068x^6 - 0.0924x^5 + 0.5039x^4 - 1.402x^3 + 2.0493x^2 - 1.3208x + 0.0051$	$y = 0.0408x^5 - 0.462x^4 + 2.0156x^3 - 4.206x^2 + 4.0986x - 1.3208$
E_{disp}	$y = 0.0025x^6 - 0.0379x^5 + 0.2156x^4 - 0.5305x^3 + 0.2408x^2 + 1.434x - 2.3567$	$y = 0.015x^5 - 0.1895x^4 + 0.8624x^3 - 1.5909x^2 + 0.4816x + 1.434$

Without the curing agent

	approximate polynomial	derivative
E_{DFT}	$y = 0.006x^6 - 0.0837x^5 + 0.4667x^4 - 1.3183x^3 + 1.9686x^2 - 1.4423x + 0.3798$	$y = 0.0408x^5 - 0.462x^4 + 2.0156x^3 - 4.206x^2 + 4.0986x - 1.3208$
E_{disp}	$y = 0.0036x^6 - 0.0509x^5 + 0.2774x^4 - 0.6758x^3 + 0.4561x^2 + 1.1401x - 2.0732$	$y = 0.0216x^5 - 0.2545x^4 + 1.1096x^3 - 2.0274x^2 + 0.9122x + 1.1401$

3. Change in surface charge with increasing CN coverage

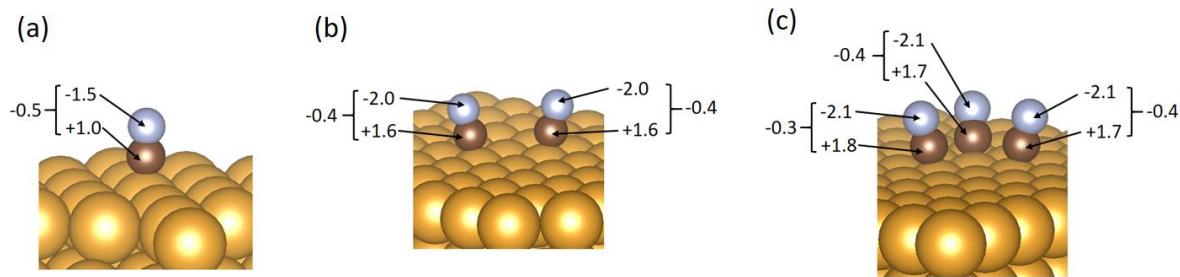


Figure S2. (a) One, (b) two, and (c) three CN groups are adsorbed on the on-top site for the 6×6 Au (111) surface slab model. The values denote the calculated Bader charges of the C and N atoms and their sum.

4. Effects of surrounding CN groups on a hydrogen bonding

When the number of CN groups on the surface increases, the hydrogen bonding between an adsorbate molecule and the CN groups should be affected. To quantify this effect, we have checked how the strength of the hydrogen bonding varies as the number of CN groups nearby. As investigated in Figure 8, we inspected the adsorption of methanol and methylamine (see Figure S3).

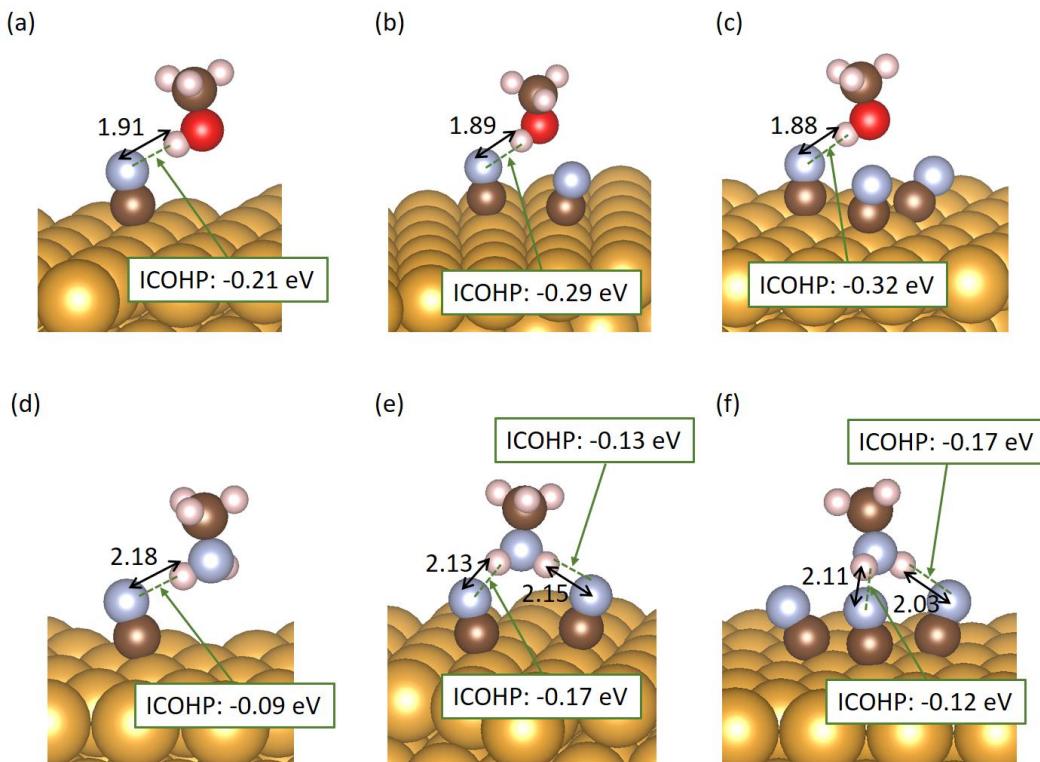


Figure S3. Interaction of methanol with (a) one, (b) two, and (c) three CN groups adsorbed on the Au surface. That of methylamine with (d) one, (e) two, and (f) three CN groups adsorbed on the surface. The values near the double-sided arrows indicate the N-H distances in Å. The ICOHP values calculated for the N ... H hydrogen bonding interactions are shown in the green-line boxes.

As the number of the CN groups increases, the number of dipole moments thereon increases. This reinforces the dipole-dipole interaction between the molecule and the surface. By and large, one can see that as the number of the CN groups increases, the molecule gets closer to the surface. This results in an increase in the orbital overlap between the H and N atoms involved in the hydrogen bonding between the CN group and the adsorbate molecule. Therefore, the magnitude of the ICOHP value increases, and one can conclude that the surrounding CN groups lead to the strengthening of the hydrogen bonding.

5. Coordinates of the optimized structures

The following structural data are provided in the VASP POSCAR format.

The initial structure of the NEB chain for the model with the curing agent

Au 5 × 5 supercell (3 layers)

1.0

14.520200000000 0.000000000000 0.000000000000
-7.260100000000 12.574862068000 0.000000000000
0.000000000000 0.000000000000 34.742300000000

Au C H N O

75 21 26 4 3

Selective dynamics

Direct

0.124235717031 0.828098794704 0.002880000000 FFFF
0.990698515218 0.962559420998 0.141149075718 TTT
0.057575717031 0.094758794704 0.071130000000 FFFF
0.457575717031 0.294758794704 0.071130000000 FFFF
0.057575717031 0.894758794704 0.071130000000 FFFF
0.992197053279 0.762662560620 0.141185559098 TTT
0.324235717031 0.828098794704 0.002880000000 FFFF
0.257575717031 0.894758794704 0.071130000000 FFFF
0.190461322815 0.762095397101 0.140820044984 TTT
0.524235717031 0.828098794704 0.002880000000 FFFF
0.457575717031 0.894758794704 0.071130000000 FFFF
0.390423210388 0.762372790831 0.141149368885 TTT
0.724235717031 0.828098794704 0.002880000000 FFFF
0.657575717031 0.894758794704 0.071130000000 FFFF
0.792308825811 0.964345663221 0.139925234767 TTT
0.924235717031 0.828098794704 0.002880000000 FFFF
0.124235717031 0.028098794704 0.002880000000 FFFF
0.793104474549 0.761507365107 0.138816880904 TTT
0.591859799155 0.762815907665 0.143474355581 TTT
0.257575717031 0.094758794704 0.071130000000 FFFF
0.057575717031 0.294758794704 0.071130000000 FFFF
0.590161919721 0.962570819099 0.140753100564 TTT
0.524235717031 0.028098794704 0.002880000000 FFFF
0.457575717031 0.094758794704 0.071130000000 FFFF
0.390180660956 0.962326810467 0.141282972690 TTT
0.724235717031 0.028098794704 0.002880000000 FFFF
0.190295672011 0.962363223891 0.141499206086 TTT

0.657575717031 0.094758794704 0.071130000000 F F F
 0.324235717031 0.028098794704 0.002880000000 F F F
 0.924235717031 0.028098794704 0.002880000000 F F F
 0.124235717031 0.228098794704 0.002880000000 F F F
 0.857575717031 0.894758794704 0.071130000000 F F F
 0.990616043075 0.162721250443 0.141100550381 T T T
 0.324235717031 0.228098794704 0.002880000000 F F F
 0.257575717031 0.294758794704 0.071130000000 F F F
 0.190071845205 0.162003372262 0.140726964500 T T T
 0.524235717031 0.228098794704 0.002880000000 F F F
 0.857575717031 0.094758794704 0.071130000000 F F F
 0.389897583715 0.162136050890 0.141436972894 T T T
 0.590226897915 0.162414411292 0.141277191866 T T T
 0.257575717031 0.694758794704 0.071130000000 F F F
 0.190539529935 0.562591723763 0.141158557026 T T T
 0.790222045621 0.162541170073 0.141286830100 T T T
 0.124235717031 0.428098794704 0.002880000000 F F F
 0.057575717031 0.494758794704 0.071130000000 F F F
 0.989912832557 0.362153549248 0.139988166701 T T T
 0.324235717031 0.428098794704 0.002880000000 F F F
 0.257575717031 0.494758794704 0.071130000000 F F F
 0.190313379352 0.362797034587 0.140836279046 T T T
 0.524235717031 0.428098794704 0.002880000000 F F F
 0.457575717031 0.494758794704 0.071130000000 F F F
 0.389186165644 0.361467846407 0.140905450973 T T T
 0.724235717031 0.428098794704 0.002880000000 F F F
 0.657575717031 0.494758794704 0.071130000000 F F F
 0.724235717031 0.228098794704 0.002880000000 F F F
 0.657575717031 0.294758794704 0.071130000000 F F F
 0.857575717031 0.294758794704 0.071130000000 F F F
 0.924235717031 0.428098794704 0.002880000000 F F F
 0.857575717031 0.494758794704 0.071130000000 F F F
 0.790217942072 0.362410374729 0.141317609799 T T T
 0.124235717031 0.628098794704 0.002880000000 F F F
 0.057575717031 0.694758794704 0.071130000000 F F F
 0.924235717031 0.228098794704 0.002880000000 F F F
 0.324235717031 0.628098794704 0.002880000000 F F F
 0.524235717031 0.628098794704 0.002880000000 F F F
 0.990251664666 0.562339343087 0.141193149444 T T T
 0.589325234024 0.361055664329 0.140693760096 T T T
 0.724235717031 0.628098794704 0.002880000000 F F F

0.657575717031 0.694758794704 0.071130000000 F F F
 0.589745963897 0.561115853403 0.139858120482 T T T
 0.924235717031 0.628098794704 0.002880000000 F F F
 0.857575717031 0.694758794704 0.071130000000 F F F
 0.790139494481 0.561679647307 0.140368174726 T T T
 0.457575717031 0.694758794704 0.071130000000 F F F
 0.389963376671 0.562529270438 0.140566612997 T T T
 0.082293496172 0.453209467282 0.235623371604 T T T
 0.351332907110 0.356791123944 0.252582815070 T T T
 0.228727038447 0.279346531808 0.309534910598 T T T
 0.198183263736 0.392189578567 0.262585358295 T T T
 0.109858907704 0.374578226941 0.240606994507 T T T
 0.254014412208 0.491098406466 0.281195982172 T T T
 0.145448563124 0.554332137449 0.251495923546 T T T
 0.727864554347 0.810754121492 0.224351438813 T T T
 0.230495471751 0.572226578740 0.275449257910 T T T
 0.162981249807 0.208008547234 0.243597780792 T T T
 0.411976183352 0.460189091645 0.237925987697 T T T
 0.747760817863 0.462745625680 0.244794369024 T T T
 0.197791885193 0.738843980438 0.248554229677 T T T
 0.571837712189 0.447677893156 0.237601204963 T T T
 0.520580053114 0.506051076233 0.231159499957 T T T
 0.511751587968 0.340595005351 0.247999820299 T T T
 0.907591447370 0.655336287245 0.244436388938 T T T
 0.842821053390 0.550239441973 0.266644368919 T T T
 0.886697828772 0.815858096012 0.238020815073 T T T
 0.403402708016 0.297600813655 0.255906305925 T T T
 0.235189038217 0.310239866215 0.266414800203 T T T
 0.250576195457 0.217645149156 0.313625067190 T T T
 0.060659960324 0.298455094880 0.226389829583 T T T
 0.207031971351 0.760038905716 0.279342640234 T T T
 0.279409616789 0.648825422911 0.289417344907 T T T
 0.147147877501 0.248260451906 0.320155443173 T T T
 0.375395041204 0.508509379269 0.232423640884 T T T
 0.321267610045 0.508151062315 0.299799643682 T T T
 0.163571408994 0.224193355401 0.212647378169 T T T
 0.080255426412 0.169564973374 0.253856178172 T T T
 0.274957735283 0.756601867278 0.236359358316 T T T
 0.170228793303 0.786160260456 0.232866964345 T T T
 0.282474434089 0.347791145395 0.327371416588 T T T
 0.191461897608 0.151088149939 0.246796857179 T T T

0.897842667581 0.520007887959 0.271954459102 TTT
 0.935865423282 0.639949180303 0.216967561311 TTT
 0.773968985991 0.437253285052 0.219086224917 TTT
 0.547487024726 0.290477062896 0.250699888524 TTT
 0.013351681119 0.437700899001 0.218255515408 TTT
 0.359794614951 0.215150931213 0.265578541866 TTT
 0.765925556825 0.597514176756 0.300486793324 TTT
 0.565959737674 0.589069935504 0.222161366926 TTT
 0.704649795928 0.394468681418 0.264139915399 TTT
 0.977244366201 0.706441754393 0.262205480302 TTT
 0.770337479201 0.662919327393 0.229708198272 TTT
 0.017328979489 0.960084061327 0.238825179652 TTT
 0.043838149254 0.858027414604 0.235161213044 TTT
 0.992628380786 0.882244423495 0.243798159634 TTT
 0.638006665710 0.773181717381 0.214057338270 TTT
 0.827618377754 0.862160771137 0.233751186350 TTT
 0.847481464044 0.710063001053 0.238080376868 TTT
 0.680461953573 0.503709860242 0.232469745221 TTT
 0.812755094110 0.568051745423 0.303887453866 TTT
 0.118600675232 0.630135880407 0.242389280822 TTT

The final structure of the NEB chain for the model with the curing agent

Au 5 × 5 supercell (3 layers)

1.0

14.520200000000 0.000000000000 0.000000000000
 -7.260100000000 12.574862068000 0.000000000000
 0.000000000000 0.000000000000 34.742300000000

Au C H N O

75 21 26 4 3

Selective dynamics

Direct

0.124235717031 0.828098794704 0.002880000000 FFF
 0.990275826537 0.962256723021 0.141053251147 TTT
 0.057575717031 0.094758794704 0.071130000000 FFF
 0.457575717031 0.294758794704 0.071130000000 FFF
 0.057575717031 0.894758794704 0.071130000000 FFF
 0.990327855923 0.762227534381 0.141002878910 TTT
 0.324235717031 0.828098794704 0.002880000000 FFF
 0.257575717031 0.894758794704 0.071130000000 FFF
 0.190353109955 0.762277823647 0.141011289968 TTT

0.524235717031 0.828098794704 0.002880000000 F F F
 0.457575717031 0.894758794704 0.071130000000 F F F
 0.390363294747 0.762350714112 0.141077833463 T T T
 0.724235717031 0.828098794704 0.002880000000 F F F
 0.657575717031 0.894758794704 0.071130000000 F F F
 0.790096056780 0.962304181825 0.140818036803 T T T
 0.924235717031 0.828098794704 0.002880000000 F F F
 0.124235717031 0.028098794704 0.002880000000 F F F
 0.790178710975 0.762146905817 0.140868487474 T T T
 0.590310243339 0.762318295214 0.141056197710 T T T
 0.257575717031 0.094758794704 0.071130000000 F F F
 0.057575717031 0.294758794704 0.071130000000 F F F
 0.590077195473 0.962321868021 0.140822163532 T T T
 0.524235717031 0.028098794704 0.002880000000 F F F
 0.457575717031 0.094758794704 0.071130000000 F F F
 0.390306239108 0.962360105630 0.141053128184 T T T
 0.724235717031 0.028098794704 0.002880000000 F F F
 0.190359886586 0.962317196544 0.141078607049 T T T
 0.657575717031 0.094758794704 0.071130000000 F F F
 0.324235717031 0.028098794704 0.002880000000 F F F
 0.924235717031 0.028098794704 0.002880000000 F F F
 0.124235717031 0.228098794704 0.002880000000 F F F
 0.857575717031 0.894758794704 0.071130000000 F F F
 0.990268945124 0.162314051725 0.141051578299 T T T
 0.324235717031 0.228098794704 0.002880000000 F F F
 0.257575717031 0.294758794704 0.071130000000 F F F
 0.190046510138 0.162245303082 0.140832031155 T T T
 0.524235717031 0.228098794704 0.002880000000 F F F
 0.857575717031 0.094758794704 0.071130000000 F F F
 0.390277764570 0.162292046175 0.141053821974 T T T
 0.590347450464 0.162381243972 0.141056800892 T T T
 0.257575717031 0.694758794704 0.071130000000 F F F
 0.190294777155 0.562381246058 0.141056928972 T T T
 0.790308439895 0.162339770787 0.141050235664 T T T
 0.124235717031 0.428098794704 0.002880000000 F F F
 0.057575717031 0.494758794704 0.071130000000 F F F
 0.990061544928 0.362323026941 0.140830191528 T T T
 0.324235717031 0.428098794704 0.002880000000 F F F
 0.257575717031 0.494758794704 0.071130000000 F F F
 0.190040873051 0.362401104017 0.140831973701 T T T
 0.524235717031 0.428098794704 0.002880000000 F F F

0.457575717031 0.494758794704 0.071130000000 F F F
 0.389955558276 0.362231275899 0.140839619087 T T T
 0.724235717031 0.428098794704 0.002880000000 F F F
 0.657575717031 0.494758794704 0.071130000000 F F F
 0.724235717031 0.228098794704 0.002880000000 F F F
 0.657575717031 0.294758794704 0.071130000000 F F F
 0.857575717031 0.294758794704 0.071130000000 F F F
 0.924235717031 0.428098794704 0.002880000000 F F F
 0.857575717031 0.494758794704 0.071130000000 F F F
 0.790277219602 0.362346429741 0.141055523904 T T T
 0.124235717031 0.628098794704 0.002880000000 F F F
 0.057575717031 0.694758794704 0.071130000000 F F F
 0.924235717031 0.228098794704 0.002880000000 F F F
 0.324235717031 0.628098794704 0.002880000000 F F F
 0.524235717031 0.628098794704 0.002880000000 F F F
 0.990348026574 0.562348432036 0.141081939469 T T T
 0.589995528516 0.362220458352 0.140842412848 T T T
 0.724235717031 0.628098794704 0.002880000000 F F F
 0.657575717031 0.694758794704 0.071130000000 F F F
 0.589997296156 0.562249420175 0.140829217141 T T T
 0.924235717031 0.628098794704 0.002880000000 F F F
 0.857575717031 0.694758794704 0.071130000000 F F F
 0.790036314188 0.562108575475 0.140868547271 T T T
 0.457575717031 0.694758794704 0.071130000000 F F F
 0.390088367684 0.562417227552 0.140831050079 T T T
 0.083660298126 0.453228471984 0.350009923613 T T T
 0.352216533706 0.356897777697 0.367964817096 T T T
 0.228690353396 0.278963517684 0.424574874769 T T T
 0.198332511918 0.391696069064 0.377652209862 T T T
 0.110838985805 0.374498249198 0.355174083293 T T T
 0.253717871144 0.490169416380 0.396531102282 T T T
 0.145575524935 0.553438321644 0.366688994570 T T T
 0.729850326805 0.810577816886 0.339078741377 T T T
 0.229861593456 0.571100855974 0.390939453357 T T T
 0.163804897716 0.207985810041 0.358276154587 T T T
 0.412744688615 0.459985828098 0.352932835684 T T T
 0.748236669623 0.462740493560 0.359632644182 T T T
 0.198324030243 0.738006760529 0.363906299136 T T T
 0.572168499862 0.447169746268 0.352431379033 T T T
 0.521023122037 0.505429344481 0.345700455490 T T T
 0.512632036778 0.340815973645 0.363933700983 T T T

0.907825159228 0.655821710452 0.359299966791 TTT
 0.843103858241 0.550631496596 0.381528337884 TTT
 0.888566001787 0.817377963960 0.352031934381 TTT
 0.404331638089 0.297925974124 0.371892008372 TTT
 0.235584957004 0.309944451868 0.381457867112 TTT
 0.250735285451 0.217427606778 0.428765339604 TTT
 0.062533648683 0.298659373707 0.340669777293 TTT
 0.207355512394 0.759279814145 0.394684527263 TTT
 0.278656355353 0.647578322110 0.404984544699 TTT
 0.147295342032 0.248072316696 0.435353976263 TTT
 0.376492907746 0.508581160948 0.347434450291 TTT
 0.321114558888 0.507190348220 0.415037228232 TTT
 0.164958304062 0.224449351317 0.327365474917 TTT
 0.081049005953 0.169327782109 0.368545385188 TTT
 0.275734197197 0.755355703916 0.352045577546 TTT
 0.171065454475 0.785831471476 0.348391146075 TTT
 0.282563236242 0.347676317328 0.442281149716 TTT
 0.192207488335 0.151096314364 0.361772454669 TTT
 0.898216815127 0.520589283633 0.386988472522 TTT
 0.936935361584 0.640231584993 0.332078818853 TTT
 0.775236758711 0.436311147036 0.334435827283 TTT
 0.548508457567 0.290881918009 0.367075767894 TTT
 0.016344186020 0.438856904997 0.331928846179 TTT
 0.360606386981 0.215522862874 0.381720370809 TTT
 0.767093955053 0.599165240486 0.415198131911 TTT
 0.565940872736 0.587669223664 0.335756683723 TTT
 0.705304683418 0.395195642665 0.379312050626 TTT
 0.977164480316 0.706452654832 0.377297504869 TTT
 0.770945717136 0.664223836482 0.344353402564 TTT
 0.020066194822 0.960510363835 0.354777645025 TTT
 0.046170426065 0.857892531532 0.351664413089 TTT
 0.994776100851 0.882464223578 0.359461811476 TTT
 0.638251723744 0.769487939314 0.331880867024 TTT
 0.832593294429 0.865090434056 0.345904920121 TTT
 0.848132778969 0.710736419776 0.352724768669 TTT
 0.680942856910 0.502600489146 0.346429813699 TTT
 0.812726809926 0.568330232914 0.418691003972 TTT
 0.118857363714 0.629579069011 0.357532612465 TTT

The initial structure of the NEB chain for the model without the curing agent

Au 5 × 5 supercell (3 layers)

1.0

12.574862068000 -7.260100000000 0.000000000000
0.000000000000 14.520200000000 0.000000000000
0.000000000000 0.000000000000 34.742277461800

Au C H O

75 19 24 3

Selective dynamics

Direct

0.133333333333 0.066666666667 0.002878337498 F F F
0.666666666667 0.733333333333 0.071127712730 F F F
0.733333333333 0.666666666667 0.002878337498 F F F
0.400673720621 0.601556812293 0.140655587223 T T T
0.466666666667 0.733333333333 0.071127712730 F F F
0.533333333333 0.666666666667 0.002878337498 F F F
0.199100013635 0.600917536227 0.140608507253 T T T
0.266666666667 0.733333333333 0.071127712730 F F F
0.333333333333 0.666666666667 0.002878337498 F F F
0.000114295190 0.601450304916 0.140934172870 T T T
0.066666666667 0.733333333333 0.071127712730 F F F
0.133333333333 0.666666666667 0.002878337498 F F F
0.800357125824 0.402099355666 0.141540180482 T T T
0.866666666667 0.533333333333 0.071127712730 F F F
0.933333333333 0.466666666667 0.002878337498 F F F
0.600571631318 0.401774379475 0.141059581273 T T T
0.133333333333 0.866666666667 0.002878337498 F F F
0.666666666667 0.533333333333 0.071127712730 F F F
0.733333333333 0.466666666667 0.002878337498 F F F
0.933333333333 0.666666666667 0.002878337498 F F F
0.466666666667 0.933333333333 0.071127712730 F F F
0.800749793418 0.802249105647 0.140898977193 T T T
0.866666666667 0.933333333333 0.071127712730 F F F
0.933333333333 0.866666666667 0.002878337498 F F F
0.600722544276 0.801648580739 0.141292993012 T T T
0.666666666667 0.933333333333 0.071127712730 F F F
0.733333333333 0.866666666667 0.002878337498 F F F
0.401233079147 0.802195655121 0.140732136947 T T T
0.533333333333 0.866666666667 0.002878337498 F F F
0.599930703789 0.601814994447 0.139662999786 T T T
0.201408335988 0.802192269685 0.139959350733 T T T
0.266666666667 0.933333333333 0.071127712730 F F F

0.333333333333 0.866666666667 0.002878337498 F F F
 0.000210396255 0.802134972774 0.140657801533 T T T
 0.801094804195 0.601726200277 0.140126164169 T T T
 0.866666666667 0.733333333333 0.071127712730 F F F
 0.400620600543 0.401760095040 0.141480021211 T T T
 0.066666666667 0.933333333333 0.071127712730 F F F
 0.533333333333 0.466666666667 0.002878337498 F F F
 0.800888105586 0.001705512141 0.141096520874 T T T
 0.866666666667 0.133333333333 0.071127712730 F F F
 0.933333333333 0.066666666667 0.002878337498 F F F
 0.600966158755 0.001926637590 0.141096536337 T T T
 0.666666666667 0.133333333333 0.071127712730 F F F
 0.733333333333 0.066666666667 0.002878337498 F F F
 0.400990698639 0.002016925653 0.141125047951 T T T
 0.466666666667 0.133333333333 0.071127712730 F F F
 0.533333333333 0.066666666667 0.002878337498 F F F
 0.200473026589 0.001410333627 0.140906738120 T T T
 0.266666666667 0.133333333333 0.071127712730 F F F
 0.333333333333 0.066666666667 0.002878337498 F F F
 0.001064397372 0.001865012823 0.141202536684 T T T
 0.066666666667 0.133333333333 0.071127712730 F F F
 0.066666666667 0.333333333333 0.071127712730 F F F
 0.466666666667 0.533333333333 0.071127712730 F F F
 0.333333333333 0.466666666667 0.002878337498 F F F
 0.133333333333 0.266666666667 0.002878337498 F F F
 0.201308014975 0.402751775830 0.140402784987 T T T
 0.266666666667 0.333333333333 0.071127712730 F F F
 0.266666666667 0.533333333333 0.071127712730 F F F
 0.999518599269 0.401741599602 0.140627913410 T T T
 0.066666666667 0.533333333333 0.071127712730 F F F
 0.133333333333 0.466666666667 0.002878337498 F F F
 0.800675625057 0.201851944803 0.141047582153 T T T
 0.333333333333 0.266666666667 0.002878337498 F F F
 0.000694723880 0.201795005564 0.140157387648 T T T
 0.866666666667 0.333333333333 0.071127712730 F F F
 0.666666666667 0.333333333333 0.071127712730 F F F
 0.733333333333 0.266666666667 0.002878337498 F F F
 0.401043785823 0.202131240327 0.141135830969 T T T
 0.466666666667 0.333333333333 0.071127712730 F F F
 0.533333333333 0.266666666667 0.002878337498 F F F
 0.201322192218 0.202249702592 0.139907499022 T T T

0.933333333333 0.266666666667 0.002878337498 F F F
 0.600862868804 0.202030935646 0.141048306324 T T T
 0.155504502416 0.693622743229 0.235016270433 T T T
 0.714377585608 0.638097597548 0.237475794469 T T T
 0.597961385469 0.551779192644 0.242021148097 T T T
 0.100131873304 0.381188118311 0.232325486890 T T T
 0.970592519947 0.645086231637 0.243696209890 T T T
 0.074124193346 0.717752285381 0.231508857282 T T T
 0.035582234964 0.529854753606 0.265802883187 T T T
 0.952069967162 0.550429464683 0.261356220437 T T T
 0.188921453836 0.103275124759 0.242088346353 T T T
 0.254655713808 0.324134033606 0.243654011406 T T T
 0.073916131283 0.275161287290 0.228392177177 T T T
 0.150109113898 0.244819635134 0.235386042595 T T T
 0.228763861131 0.573495521881 0.257833363443 T T T
 0.332335227552 0.657799554235 0.238417653309 T T T
 0.201292815095 0.460626250338 0.244661698633 T T T
 0.138430467675 0.598150872665 0.251647056116 T T T
 0.278008724035 0.429066956594 0.248575212504 T T T
 0.249518631660 0.578882665180 0.301992491376 T T T
 0.788051314802 0.597291300705 0.249249798988 T T T
 0.784605635892 0.585492493364 0.280734509831 T T T
 0.579253611871 0.480595844055 0.224981908830 T T T
 0.234229250760 0.752385233545 0.224650353500 T T T
 0.090057745957 0.793695040443 0.219422991918 T T T
 0.762794454117 0.520482860518 0.234842177847 T T T
 0.019037685243 0.457628985344 0.281096346994 T T T
 0.730703620409 0.661004205646 0.206737536693 T T T
 0.727562506671 0.778720525872 0.244691998436 T T T
 0.579290116952 0.529028678905 0.272418218917 T T T
 0.257176066596 0.136792033400 0.222167896543 T T T
 0.873850806076 0.492960973891 0.272274372697 T T T
 0.545993646749 0.581413622873 0.231762740305 T T T
 0.318038516873 0.305446902870 0.247191631751 T T T
 0.179961419387 0.516613569865 0.317273937241 T T T
 0.317787833855 0.568246847218 0.308363745294 T T T
 0.144303366268 0.016725647439 0.238657724786 T T T
 0.038353813603 0.400605980985 0.226041486887 T T T
 0.993192143634 0.214122351075 0.220724352631 T T T
 0.359422665169 0.487251075153 0.256544327335 T T T
 0.266507956030 0.656708393779 0.313137761138 T T T

```

0.360796191405 0.737283753016 0.250712394910 TTT
0.320906868193 0.661910197390 0.207273865680 TTT
0.396311390127 0.639129894549 0.241998204740 TTT
0.217641941969 0.123828028653 0.271927942218 TTT
0.894653990452 0.672709006500 0.237708865710 TTT
0.739214571679 0.729909503520 0.260322547649 TTT
0.115288501126 0.138447726463 0.233088166298 TTT

```

The final structure of the NEB chain for the model without the curing agent

Au 5 × 5 supercell (3 layers)

1.0

```

12.574862068000 -7.260100000000 0.000000000000
0.000000000000 14.520200000000 0.000000000000
0.000000000000 0.000000000000 34.742277461800

```

Au C H O

75 19 24 3

Selective dynamics

Direct

```

0.133333333333 0.066666666667 0.002878337498 FFF
0.666666666667 0.733333333333 0.071127712730 FFF
0.733333333333 0.666666666667 0.002878337498 FFF
0.401009450434 0.601958012814 0.140953064269 TTT
0.466666666667 0.733333333333 0.071127712730 FFF
0.533333333333 0.666666666667 0.002878337498 FFF
0.201038436226 0.601979978680 0.140940464824 TTT
0.266666666667 0.733333333333 0.071127712730 FFF
0.333333333333 0.666666666667 0.002878337498 FFF
0.001100204833 0.602050815837 0.140923224279 TTT
0.066666666667 0.733333333333 0.071127712730 FFF
0.133333333333 0.666666666667 0.002878337498 FFF
0.801018238931 0.401945559755 0.140933884403 TTT
0.866666666667 0.533333333333 0.071127712730 FFF
0.933333333333 0.466666666667 0.002878337498 FFF
0.600927681786 0.401917557283 0.140933395014 TTT
0.133333333333 0.866666666667 0.002878337498 FFF
0.666666666667 0.533333333333 0.071127712730 FFF
0.733333333333 0.466666666667 0.002878337498 FFF
0.933333333333 0.666666666667 0.002878337498 FFF
0.466666666667 0.933333333333 0.071127712730 FFF
0.801116466374 0.801820828896 0.140951817871 TTT

```

0.8666666666667 0.933333333333 0.071127712730 F F F
 0.933333333333 0.8666666666667 0.002878337498 F F F
 0.601071646329 0.801807391521 0.140931209104 T T T
 0.6666666666667 0.933333333333 0.071127712730 F F F
 0.733333333333 0.8666666666667 0.002878337498 F F F
 0.401111157762 0.801985698311 0.140926505751 T T T
 0.533333333333 0.8666666666667 0.002878337498 F F F
 0.601055741910 0.601773687460 0.141061406419 T T T
 0.201157852245 0.801895636153 0.141060786332 T T T
 0.2666666666667 0.933333333333 0.071127712730 F F F
 0.333333333333 0.8666666666667 0.002878337498 F F F
 0.001293465913 0.801895829074 0.140957430134 T T T
 0.801073422785 0.601878158680 0.140993594510 T T T
 0.8666666666667 0.733333333333 0.071127712730 F F F
 0.401017966001 0.401929282619 0.140975145366 T T T
 0.0666666666667 0.933333333333 0.071127712730 F F F
 0.533333333333 0.4666666666667 0.002878337498 F F F
 0.801232326351 0.001828267278 0.140945388099 T T T
 0.8666666666667 0.133333333333 0.071127712730 F F F
 0.933333333333 0.0666666666667 0.002878337498 F F F
 0.601278138379 0.001808946209 0.140898300710 T T T
 0.6666666666667 0.133333333333 0.071127712730 F F F
 0.733333333333 0.0666666666667 0.002878337498 F F F
 0.401257478205 0.001861485269 0.140952759494 T T T
 0.4666666666667 0.133333333333 0.071127712730 F F F
 0.533333333333 0.0666666666667 0.002878337498 F F F
 0.201253053589 0.001971971511 0.140946232775 T T T
 0.2666666666667 0.133333333333 0.071127712730 F F F
 0.333333333333 0.0666666666667 0.002878337498 F F F
 0.001036278570 0.001970708800 0.140956971634 T T T
 0.0666666666667 0.133333333333 0.071127712730 F F F
 0.0666666666667 0.333333333333 0.071127712730 F F F
 0.4666666666667 0.533333333333 0.071127712730 F F F
 0.333333333333 0.4666666666667 0.002878337498 F F F
 0.133333333333 0.2666666666667 0.002878337498 F F F
 0.200982035476 0.401966974216 0.140931653301 T T T
 0.2666666666667 0.333333333333 0.071127712730 F F F
 0.2666666666667 0.533333333333 0.071127712730 F F F
 1.000966500000 0.401961392773 0.140970532383 T T T
 0.0666666666667 0.533333333333 0.071127712730 F F F
 0.133333333333 0.4666666666667 0.002878337498 F F F

0.801141680205 0.201914500702 0.140934861167 TTT
 0.333333333333 0.266666666667 0.002878337498 FFF
 0.001239861957 0.201956088619 0.141007399705 TTT
 0.866666666667 0.333333333333 0.071127712730 FFF
 0.666666666667 0.333333333333 0.071127712730 FFF
 0.733333333333 0.266666666667 0.002878337498 FFF
 0.401050688330 0.201927062421 0.140925786477 TTT
 0.466666666667 0.333333333333 0.071127712730 FFF
 0.533333333333 0.266666666667 0.002878337498 FFF
 0.201047904900 0.201813946472 0.141029877235 TTT
 0.933333333333 0.266666666667 0.002878337498 FFF
 0.601084016389 0.201929775948 0.140904169679 TTT
 0.145096081416 0.672584641036 0.342497551623 TTT
 0.712905843492 0.634601676094 0.350930190108 TTT
 0.594777246092 0.550818631361 0.353487664062 TTT
 0.106516318892 0.385696216871 0.343640906578 TTT
 0.965354568414 0.633068938757 0.356541801452 TTT
 0.062193945820 0.693489107971 0.337236919839 TTT
 0.038555432242 0.533199714011 0.386638998876 TTT
 0.953842048889 0.551963946591 0.381513829976 TTT
 0.179962260750 0.097264260136 0.351209056191 TTT
 0.246023165909 0.315091285762 0.364489784493 TTT
 0.081315010007 0.281936513517 0.335317140503 TTT
 0.149809939632 0.244811541553 0.346314098797 TTT
 0.228199656849 0.570577175894 0.374552244437 TTT
 0.328663752936 0.648573833676 0.351697340353 TTT
 0.199762928080 0.456293570106 0.363542510227 TTT
 0.136045532214 0.592046915832 0.367310507224 TTT
 0.269228867687 0.418630145598 0.372872292553 TTT
 0.255796765687 0.589530579833 0.418079845434 TTT
 0.783719334329 0.591004203390 0.363979282093 TTT
 0.784130297622 0.588917402895 0.395766084417 TTT
 0.574418034735 0.483664110203 0.333959898798 TTT
 0.218606171475 0.721098932175 0.326666219771 TTT
 0.071029907921 0.756481839297 0.317901964931 TTT
 0.753301215572 0.509546172321 0.352896295826 TTT
 0.027052474012 0.469516368921 0.406273708572 TTT
 0.733984011538 0.661251266135 0.320770898691 TTT
 0.714672848174 0.768690973042 0.362817478329 TTT
 0.573072540184 0.520106469660 0.383023147208 TTT
 0.255104171804 0.131106148872 0.334892159866 TTT

0.880029283717 0.503310072625 0.397173418204 TTT
 0.545608539865 0.585732654517 0.345315723605 TTT
 0.303170226420 0.290589848149 0.372409545497 TTT
 0.190035152080 0.531748655233 0.436044966604 TTT
 0.326280835657 0.583250715978 0.425000340194 TTT
 0.132988284464 0.011459668213 0.345846015315 TTT
 0.051038399153 0.411650688951 0.334847544965 TTT
 1.007692800000 0.227599479316 0.320478957835 TTT
 0.344643689698 0.470849316572 0.387251295809 TTT
 0.272513790705 0.669518396101 0.426285186304 TTT
 0.356364189929 0.731654584719 0.359803610632 TTT
 0.314568852426 0.639925674873 0.320487912309 TTT
 0.393549853683 0.632562032811 0.357941215183 TTT
 0.197460107702 0.111347107398 0.382220011742 TTT
 0.888666414952 0.659481737907 0.349357183233 TTT
 0.738700489776 0.724583142372 0.375327276886 TTT
 0.115591155455 0.140136552225 0.338433059624 TTT

Optimized 6x6 Au(111) surface with 100% coverage of CN

1.000000000000000
 17.3028000000000013 0.000000000000000 0.000000000000000
 -8.6514000000000006 14.9846643565999997 0.000000000000000
 0.000000000000000 0.000000000000000 34.7092000000000027

Au C N

108 36 36

Selective dynamics

Direct

0.0000028908449750 0.0000070376909633 0.1372981060992373 T T T
 0.0000038753291705 0.5000156749106353 0.1371710522990668 T T T
 0.4444400000000002 0.7222200000000001 0.0678399999999968 F F F
 0.3333362480543727 0.6666814169045097 0.1371679884471391 T T T
 0.2222200000000001 0.7777799999999999 0.000000000000000 F F F
 0.2777799999999999 0.7222200000000001 0.0678399999999968 F F F
 0.1666637802220166 0.6666826582780203 0.1371685524513140 T T T
 0.0555599999999998 0.7777799999999999 0.000000000000000 F F F
 0.1111099999999965 0.7222200000000001 0.0678399999999968 F F F
 0.9999866032763336 0.6666818331531701 0.1372848719175366 T T T
 0.8888900000000035 0.6111099999999965 0.000000000000000 F F F
 0.9444400000000002 0.5555599999999998 0.0678399999999968 F F F
 0.8333465377326590 0.5000327558716933 0.1372847867200093 T T T
 0.7222200000000001 0.6111099999999965 0.000000000000000 F F F

0.7777799999999999 0.5555599999999998 0.0678399999999968 F F F
 0.6666899076279833 0.5000225559229960 0.1372817552523955 T T T
 0.6111099999999965 0.5555599999999998 0.0678399999999968 F F F
 0.3888900000000035 0.6111099999999965 0.0000000000000000 F F F
 0.4444400000000002 0.5555599999999998 0.0678399999999968 F F F
 0.3333535693111784 0.5000141240114147 0.1371843834493234 T T T
 0.2222200000000001 0.6111099999999965 0.0000000000000000 F F F
 0.2777799999999999 0.5555599999999998 0.0678399999999968 F F F
 0.1666797426269824 0.5000151866205940 0.1371918210419665 T T T
 0.0555599999999998 0.6111099999999965 0.0000000000000000 F F F
 0.3888900000000035 0.7777799999999999 0.0000000000000000 F F F
 0.5000041293827309 0.6666763524629431 0.1371684904966060 T T T
 0.5000237769251967 0.5000197959554242 0.1372839894245459 T T T
 0.5555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.8888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.4999954807742952 0.8333504862349486 0.1371937959399929 T T T
 0.6111099999999965 0.8888900000000035 0.0678399999999968 F F F
 0.5555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.9444400000000002 0.8888900000000035 0.0678399999999968 F F F
 0.6666660011726435 0.8333485052057341 0.1371717957911542 T T T
 0.7777799999999999 0.8888900000000035 0.0678399999999968 F F F
 0.7222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.8333320653816969 0.8333589726348194 0.1372811139422794 T T T
 0.4444400000000002 0.8888900000000035 0.0678399999999968 F F F
 0.3888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.2222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.7222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.3333323673845854 0.8333585284349851 0.1371864720316580 T T T
 0.2777799999999999 0.8888900000000035 0.0678399999999968 F F F
 0.1666602192320426 0.8333443606559641 0.1371773588979366 T T T
 0.0555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.1111099999999965 0.8888900000000035 0.0678399999999968 F F F
 0.8888900000000035 0.7777799999999999 0.0000000000000000 F F F
 0.9444400000000002 0.7222200000000001 0.0678399999999968 F F F
 0.8333261047835592 0.6666900519401082 0.1372825253350243 T T T
 0.6111099999999965 0.7222200000000001 0.0678399999999968 F F F
 0.7777799999999999 0.7222200000000001 0.0678399999999968 F F F
 0.6666701036498210 0.6666770193072864 0.1371674551305446 T T T
 0.1111099999999965 0.5555599999999998 0.0678399999999968 F F F
 0.6111099999999965 0.3888900000000035 0.0678399999999968 F F F
 0.9999821318606479 0.8333379466001887 0.1371695983223802 T T T

0.8333630905101757 0.3333571155342341 0.1372573057067612 T T T
 0.3333575407881568 0.1666834493094456 0.1371754147993585 T T T
 0.2222200000000001 0.2777799999999999 0.0000000000000000 F F F
 0.2777799999999999 0.22220000000001 0.067839999999968 F F F
 0.1666844235702243 0.1666762227661565 0.1371750404623668 T T T
 0.0555599999999998 0.2777799999999999 0.0000000000000000 F F F
 0.0000148950378858 0.1666619873028949 0.1371739584762466 T T T
 0.8888900000000035 0.1111099999999965 0.0000000000000000 F F F
 0.9444400000000002 0.0555599999999998 0.067839999999968 F F F
 0.8888900000000035 0.4444400000000002 0.0000000000000000 F F F
 0.7222200000000001 0.1111099999999965 0.0000000000000000 F F F
 0.4444400000000002 0.2222200000000001 0.067839999999968 F F F
 0.7777799999999999 0.0555599999999998 0.067839999999968 F F F
 0.5555599999999998 0.1111099999999965 0.0000000000000000 F F F
 0.6111099999999965 0.0555599999999998 0.067839999999968 F F F
 0.5000002738172924 0.0000231017666863 0.1371676251486491 T T T
 0.3888900000000035 0.1111099999999965 0.0000000000000000 F F F
 0.4444400000000002 0.0555599999999998 0.067839999999968 F F F
 0.3333334114733120 0.0000224587117401 0.1372745400319815 T T T
 0.2222200000000001 0.1111099999999965 0.0000000000000000 F F F
 0.2777799999999999 0.0555599999999998 0.067839999999968 F F F
 0.1666618405816678 0.0000075694136967 0.1371659277752286 T T T
 0.0555599999999998 0.1111099999999965 0.0000000000000000 F F F
 0.5555599999999998 0.6111099999999965 0.0000000000000000 F F F
 0.1111099999999965 0.0555599999999998 0.067839999999968 F F F
 0.6666744884612896 0.0000150858169974 0.1371701312134945 T T T
 0.1111099999999965 0.2222200000000001 0.067839999999968 F F F
 0.8333436899907056 0.0000077693721678 0.1372746158507141 T T T
 0.6111099999999965 0.2222200000000001 0.067839999999968 F F F
 0.5000244741310880 0.1666905198588964 0.1371729347257613 T T T
 0.7222200000000001 0.4444400000000002 0.0000000000000000 F F F
 0.7777799999999999 0.3888900000000035 0.067839999999968 F F F
 0.6667032586034409 0.3333577024876249 0.1371734431306137 T T T
 0.3888900000000035 0.2777799999999999 0.0000000000000000 F F F
 0.5000328382893073 0.3333679824742646 0.1371746137989476 T T T
 0.3888900000000035 0.4444400000000002 0.0000000000000000 F F F
 0.4444400000000002 0.3888900000000035 0.067839999999968 F F F
 0.3333584838928161 0.3333529804614912 0.1371790266017996 T T T
 0.2222200000000001 0.4444400000000002 0.0000000000000000 F F F
 0.1666866017774211 0.3333462280943635 0.1371775641989004 T T T
 0.9444400000000002 0.3888900000000035 0.067839999999968 F F F

0.5555599999999998 0.4444400000000002 0.0000000000000000 F F F
 0.6666992222675105 0.1666869578057231 0.1371867296357294 T T T
 0.5555599999999998 0.2777799999999999 0.0000000000000000 F F F
 0.8888900000000035 0.2777799999999999 0.0000000000000000 F F F
 0.0555599999999998 0.4444400000000002 0.0000000000000000 F F F
 0.2777799999999999 0.3888900000000035 0.0678399999999968 F F F
 0.0000229383912114 0.3333437896401037 0.1371752442929548 T T T
 0.1111099999999965 0.3888900000000035 0.0678399999999968 F F F
 0.9444400000000002 0.2222200000000001 0.0678399999999968 F F F
 0.8333591467516754 0.1666774008886307 0.1371857746721261 T T T
 0.7777799999999999 0.2222200000000001 0.0678399999999968 F F F
 0.7222200000000001 0.2777799999999999 0.0000000000000000 F F F
 0.6688719583202456 0.5035632924646691 0.195518120364871 T T T
 0.6684781397952051 0.0035126480257333 0.1953611247659524 T T T
 0.8360526005207518 0.1702045321622947 0.1953893851916320 T T T
 0.0012597342152887 0.8368746665664446 0.1953646509628300 T T T
 0.8353124202736382 0.0035877452300710 0.1954978711259443 T T T
 0.8347175304302112 0.6702123728174811 0.1955163166754517 T T T
 0.1695007586981134 0.1702230477196949 0.1953690455294037 T T T
 0.6693830989254579 0.1701957238923981 0.1953929961443279 T T T
 0.0028225890473408 0.3368833244680900 0.1953697723513770 T T T
 0.5013042592143577 0.8368666615654874 0.1954069528323004 T T T
 0.8355268143870873 0.5035663684308815 0.1955191826884359 T T T
 0.1683073714988694 0.6701378571729180 0.1953601703106926 T T T
 0.3357068013922486 0.5035259667002023 0.1953911023647521 T T T
 0.3351158379522090 0.0035177189998876 0.1955021591849899 T T T
 0.5028368003128492 0.3368623907311843 0.1953714495740257 T T T
 0.8346355474809783 0.8369162083494501 0.1955121487632354 T T T
 0.6681152255930982 0.6702033680178445 0.1953639377036893 T T T
 0.6679786419767595 0.8368866929340726 0.1953683746449215 T T T
 0.1684944961562707 0.0034726343049130 0.1953600794513548 T T T
 0.1678948566648302 0.8368161298140890 0.1953768472933959 T T T
 0.3345797559811103 0.8368541371925389 0.1953938556783044 T T T
 0.5017097472183778 0.0034721820052752 0.1953602592219141 T T T
 0.8361378394368160 0.3368829006888276 0.1954676047785071 T T T
 0.0020788626279753 0.0035971057330642 0.1955438292065850 T T T
 0.5027697465285286 0.1701893141951487 0.1953681598322063 T T T
 0.0027541051942492 0.1702190211032857 0.1953670160094063 T T T
 0.3361761495377280 0.3368645948385591 0.1953774168025078 T T T
 0.3361351326961852 0.1701960379044891 0.1953698311737497 T T T
 0.6695022737767005 0.3368824842251783 0.1953703669796880 T T T

0.5016365194996695 0.6701448475527627 0.1953613456892640 T T T
 0.5022846726661072 0.5035002882063608 0.1955236902726867 T T T
 0.1690151474625381 0.5035322478079181 0.1954029811324389 T T T
 0.0022895175965800 0.5035505040911517 0.1953648995524517 T T T
 0.3349808814106865 0.6701381581344492 0.1953610371658101 T T T
 0.0013758803519437 0.6701472668206989 0.1955182382824887 T T T
 0.1695109123442080 0.3368735905906348 0.1953731183473479 T T T
 0.8365939246524476 0.5053659426592674 0.2294274018986329 T T T
 0.6689328303903324 0.6720694462033237 0.2292708463998210 T T T
 0.1695165700738386 0.0052588182432629 0.2292680400975158 T T T
 0.3368872294426026 0.5052181508731977 0.2292984923998844 T T T
 0.0029906743024881 0.0054538996477049 0.2294523603408010 T T T
 0.8362694891814044 0.0054596994349723 0.2294056229278851 T T T
 0.0041477750799643 0.3386873057223312 0.2292754407588404 T T T
 0.6704964882457887 0.1719261106869041 0.2293000985420193 T T T
 0.1690123356567952 0.6718176342138307 0.2292687755394738 T T T
 0.0040342992842497 0.1720866857166854 0.2292732107778264 T T T
 0.3359807785382287 0.0051279669214850 0.2294118999570287 T T T
 0.3376583283131112 0.3385903800065648 0.2292832809634362 T T T
 0.1708309307186724 0.1720725450175848 0.2292741815593331 T T T
 0.1709397698031978 0.3386783290528399 0.2292778934003081 T T T
 0.5025652270610550 0.0051371745533899 0.2292690492302185 T T T
 0.3374290288138653 0.1719164535212627 0.2292763465124210 T T T
 0.5018893550336614 0.8385991202379870 0.2293144591879539 T T T
 0.8353159877859326 0.8387725095848140 0.2294200301463221 T T T
 0.0018527194850435 0.8386144906388111 0.2292737338466679 T T T
 0.5039339491316071 0.1718383785740230 0.2292756334759574 T T T
 0.6699172603662760 0.5053419177300356 0.2294264911301767 T T T
 0.5034066463916744 0.5052446582029475 0.2294319238189715 T T T
 0.1701795841182090 0.5052402354908239 0.2293103020653859 T T T
 0.5042801170584283 0.3385788123074889 0.2292770512072266 T T T
 0.5023980342133427 0.6719773320362137 0.2292685091545223 T T T
 0.0021815180132521 0.6718798605063867 0.2294269373351057 T T T
 0.1684350657087705 0.8384160689195070 0.2292861471591650 T T T
 0.3351284477660741 0.8384497898790571 0.2293031475830318 T T T
 0.6686728749906266 0.8388013808877446 0.2292747060022364 T T T
 0.0033879100470315 0.5053421267439688 0.2292715028441492 T T T
 0.3357811890119180 0.6718562178645655 0.2292687187942590 T T T
 0.8374513288598493 0.3387183244159004 0.2293735189566988 T T T
 0.6708855012538564 0.3387198601816550 0.2292757606052405 T T T
 0.8371827390262681 0.1720077498092394 0.2292960229946033 T T T

```

0.6693636583386748 0.0052987484162230 0.2292678226201730 T T T
0.8354755226215573 0.6719705917137517 0.2294253101035295 T T T

```

The initial structure of the NEB chain for the model with the curing agent (coverage: 0 %)

Au 6 × 6 supercell (3 layers)

1.0

```

17.302800000000 0.000000000000 0.000000000000
-8.651400000000 14.984664356600 0.000000000000
0.000000000000 0.000000000000 34.709200000000

```

Au C H N O

108 21 26 4 3

Selective dynamics

Direct

```

0.974596282918 0.978542471743 0.142406106446 TTT
0.308346712696 0.645316804332 0.140304357354 TTT
0.196980000000 0.755800000000 0.001480000000 FFF
0.252090000000 0.700540000000 0.071430000000 FFF
0.141957505223 0.645698811157 0.142339008248 TTT
0.030310000000 0.755840000000 0.001580000000 FFF
0.086140000000 0.700020000000 0.070430000000 FFF
0.975932584053 0.645538916909 0.139698396113 TTT
0.863790000000 0.588980000000 0.002150000000 FFF
0.919090000000 0.533120000000 0.071610000000 FFF
0.808350148836 0.479506789184 0.142370398424 TTT
0.752830000000 0.533710000000 0.071220000000 FFF
0.475003311351 0.645404446851 0.139093376812 TTT
0.642402305041 0.479174725635 0.140371798960 TTT
0.530050000000 0.589080000000 0.001240000000 FFF
0.585540000000 0.533210000000 0.070300000000 FFF
0.475170952184 0.479158214680 0.140825743351 TTT
0.363100000000 0.588970000000 0.001810000000 FFF
0.418740000000 0.533200000000 0.070580000000 FFF
0.308503553380 0.479095052741 0.142091383038 TTT
0.196540000000 0.588830000000 0.002950000000 FFF
0.252360000000 0.533350000000 0.071860000000 FFF
0.030150000000 0.588540000000 0.002300000000 FFF
0.418730000000 0.700590000000 0.070570000000 FFF
0.974428299341 0.479230145941 0.142507807374 TTT
0.585890000000 0.700610000000 0.070280000000 FFF
0.141501718749 0.479212952292 0.142429314538 TTT

```

0.029980000000 0.922770000000 0.002560000000 F F F
 0.418980000000 0.866930000000 0.071690000000 F F F
 0.863530000000 0.922730000000 0.003450000000 F F F
 0.918990000000 0.866770000000 0.072200000000 F F F
 0.807987328000 0.811939882999 0.142254328558 T T T
 0.697080000000 0.922670000000 0.003600000000 F F F
 0.752290000000 0.866490000000 0.072540000000 F F F
 0.641057374019 0.811357169052 0.142349786766 T T T
 0.530550000000 0.922650000000 0.003160000000 F F F
 0.585690000000 0.866680000000 0.072310000000 F F F
 0.475451327787 0.812030661510 0.141302508962 T T T
 0.363980000000 0.922700000000 0.001990000000 F F F
 0.196860000000 0.922600000000 0.001880000000 F F F
 0.308892682546 0.811541461383 0.141370547717 T T T
 0.253170000000 0.867290000000 0.070550000000 F F F
 0.142310137773 0.811693705879 0.139798332355 T T T
 0.530260000000 0.756230000000 0.001760000000 F F F
 0.085480000000 0.867120000000 0.070870000000 F F F
 0.975331845949 0.811987800951 0.141149732732 T T T
 0.863890000000 0.756160000000 0.002120000000 F F F
 0.919460000000 0.700540000000 0.071000000000 F F F
 0.808832219333 0.645754605228 0.140400549043 T T T
 0.697280000000 0.756220000000 0.001970000000 F F F
 0.752920000000 0.700390000000 0.070970000000 F F F
 0.641507704151 0.645257279486 0.139652346796 T T T
 0.085800000000 0.533770000000 0.072730000000 F F F
 0.530500000000 0.088930000000 0.003010000000 F F F
 0.697130000000 0.589150000000 0.001710000000 F F F
 0.141442988708 0.312460397981 0.142416569270 T T T
 0.863550000000 0.421960000000 0.002990000000 F F F
 0.306967000761 0.144936512855 0.141629006289 T T T
 0.141153597433 0.145448393058 0.142397347536 T T T
 0.029990000000 0.255660000000 0.003890000000 F F F
 0.085720000000 0.200180000000 0.072890000000 F F F
 0.974378154331 0.145381924563 0.142540548253 T T T
 0.863480000000 0.089200000000 0.004000000000 F F F
 0.918890000000 0.033400000000 0.072980000000 F F F
 0.807433484959 0.978369514219 0.142533057898 T T T
 0.697110000000 0.089160000000 0.003920000000 F F F
 0.752250000000 0.033330000000 0.073220000000 F F F
 0.363150000000 0.255160000000 0.002540000000 F F F

0.418990000000 0.199750000000 0.071750000000 F F F
 0.585870000000 0.033380000000 0.072790000000 F F F
 0.475474716349 0.978183189799 0.141426561328 T T T
 0.363460000000 0.088800000000 0.002680000000 F F F
 0.419220000000 0.033340000000 0.071830000000 F F F
 0.307612650506 0.977704033852 0.140595920306 T T T
 0.196550000000 0.088960000000 0.003040000000 F F F
 0.252140000000 0.033160000000 0.071820000000 F F F
 0.141272963890 0.978057732441 0.142118044994 T T T
 0.029960000000 0.089210000000 0.003620000000 F F F
 0.085570000000 0.033420000000 0.072450000000 F F F
 0.363340000000 0.756020000000 0.001980000000 F F F
 0.641092496912 0.978258712137 0.143486355612 T T T
 0.252380000000 0.199980000000 0.072280000000 F F F
 0.196520000000 0.255470000000 0.003380000000 F F F
 0.473776952856 0.144612549806 0.144175170621 T T T
 0.807526229373 0.312510775064 0.142825015978 T T T
 0.697020000000 0.422200000000 0.002280000000 F F F
 0.752570000000 0.367040000000 0.072090000000 F F F
 0.641433996075 0.312895554458 0.139465815311 T T T
 0.529920000000 0.421970000000 0.001570000000 F F F
 0.585630000000 0.366780000000 0.071000000000 F F F
 0.474414671052 0.313601084982 0.139868116795 T T T
 0.363000000000 0.421890000000 0.002100000000 F F F
 0.418780000000 0.366430000000 0.071160000000 F F F
 0.308067586258 0.312387136189 0.142245614948 T T T
 0.196500000000 0.422030000000 0.003230000000 F F F
 0.919070000000 0.367050000000 0.073130000000 F F F
 0.252540000000 0.366810000000 0.072360000000 F F F
 0.974395235020 0.312420424860 0.142783232616 T T T
 0.863540000000 0.255670000000 0.004050000000 F F F
 0.919000000000 0.200260000000 0.073240000000 F F F
 0.807660337743 0.145447766376 0.142876243327 T T T
 0.697000000000 0.255520000000 0.003250000000 F F F
 0.752320000000 0.200340000000 0.073140000000 F F F
 0.641635008327 0.145594619589 0.142286350193 T T T
 0.530100000000 0.255260000000 0.002420000000 F F F
 0.585620000000 0.199780000000 0.072020000000 F F F
 0.030080000000 0.422160000000 0.003880000000 F F F
 0.085830000000 0.366990000000 0.073000000000 F F F
 0.605535948415 0.583546111336 0.251937164704 T T T

0.620150522925 0.377060102422 0.239872291885 TTT
 0.567272949082 0.483998217102 0.244657712489 TTT
 0.511474146382 0.232693402180 0.227200621670 TTT
 0.899448305539 0.642705229204 0.239711369118 TTT
 0.513847058721 0.733110173218 0.242103806762 TTT
 0.423314793868 0.680233172182 0.233346758974 TTT
 0.367232534565 0.716810759969 0.235182204446 TTT
 0.490866943936 0.858157464024 0.252336001391 TTT
 0.534068044225 0.606786016759 0.241779636354 TTT
 0.335923700679 0.841072396670 0.259309172979 TTT
 0.047582542088 0.665853200817 0.244135603759 TTT
 0.345357810397 0.853354362921 0.303925101311 TTT
 0.236014626491 0.777727254418 0.251481294009 TTT
 0.181827409764 0.809301229530 0.236406752391 TTT
 0.397734210224 0.804626646350 0.247104353683 TTT
 0.191396012752 0.687813815247 0.263625284366 TTT
 0.368065559588 0.933579755654 0.241415981633 TTT
 0.088942253758 0.755673180602 0.233403774612 TTT
 0.100033128237 0.632046961174 0.258960145804 TTT
 0.548447245487 0.824136155981 0.249469869546 TTT
 0.509618594766 0.584175554166 0.212135741297 TTT
 0.619986671411 0.866926727262 0.254103172018 TTT
 0.067464278628 0.562353365320 0.267913336416 TTT
 0.297474689343 0.673667276082 0.227575576403 TTT
 0.698587129990 0.693639221649 0.227159708533 TTT
 0.750634761177 0.413358949546 0.227703957859 TTT
 0.477571909453 0.572965255487 0.262002080068 TTT
 0.515931874363 0.445094814973 0.266252564453 TTT
 0.700165386930 0.512450669577 0.241284030033 TTT
 0.675925250141 0.301579473585 0.226016385509 TTT
 0.534959524041 0.466326448964 0.216052509745 TTT
 0.624111720439 0.599267709969 0.282663677742 TTT
 0.394421190494 0.610311585728 0.225448302167 TTT
 0.327203927557 0.790160831582 0.318476825478 TTT
 0.356894911488 0.929551002166 0.210087163150 TTT
 0.228248681813 0.659937830978 0.277755940922 TTT
 0.914969278939 0.689082129050 0.215441919954 TTT
 0.050374614497 0.785485804396 0.222972209739 TTT
 0.439565829702 0.978388065607 0.246049260038 TTT
 0.334196229422 0.966714272342 0.254180443944 TTT
 0.210997244730 0.878515915211 0.227377185463 TTT

```

0.301216445502 0.877417185407 0.314497918620 TTT
0.414334631529 0.902296055651 0.311874685709 TTT
0.519931500438 0.928570192922 0.259699400087 TTT
0.832629072270 0.585908592542 0.234514489546 TTT
0.900573220315 0.675982746627 0.266951128497 TTT
0.690003493546 0.362527085550 0.235957658146 TTT
0.483594791230 0.159446359449 0.214770873873 TTT
0.534834110483 0.312437820979 0.239138637392 TTT
0.637476483145 0.461125257963 0.246418255830 TTT
0.684361530757 0.631551862489 0.228811137505 TTT
0.572348379410 0.701136060723 0.244631629743 TTT
0.957537684455 0.606478427812 0.241533334727 TTT

```

The final structure of the NEB chain for the model with the curing agent (coverage: 0 %)

Au 6 × 6 supercell (3 layers)

1.0

```

17.302800000000 0.000000000000 0.000000000000
-8.651400000000 14.984664356600 0.000000000000
0.000000000000 0.000000000000 34.709200000000

```

Au C H N O

108 21 26 4 3

Selective dynamics

Direct

```

0.975070987516 0.978810291457 0.142278913345 TTT
0.309425489926 0.645477059950 0.141082761197 TTT
0.196980000000 0.755800000000 0.001480000000 FFF
0.252090000000 0.700540000000 0.071430000000 FFF
0.142672749543 0.645812065483 0.141507501906 TTT
0.030310000000 0.755840000000 0.001580000000 FFF
0.086140000000 0.700020000000 0.070430000000 FFF
0.976088362330 0.645787825365 0.140777557212 TTT
0.863790000000 0.588980000000 0.002150000000 FFF
0.919090000000 0.533120000000 0.071610000000 FFF
0.808440852716 0.479111006708 0.141666746556 TTT
0.752830000000 0.533710000000 0.071220000000 FFF
0.475805992062 0.645048400930 0.140256640024 TTT
0.642351049927 0.478880736844 0.140672675326 TTT
0.530050000000 0.589080000000 0.001240000000 FFF
0.585540000000 0.533210000000 0.070300000000 FFF
0.475923577797 0.478706344770 0.140604869974 TTT

```

0.363100000000 0.588970000000 0.001810000000 F F F
 0.418740000000 0.533200000000 0.070580000000 F F F
 0.309376974912 0.479073022671 0.141474149264 T T T
 0.196540000000 0.588830000000 0.002950000000 F F F
 0.252360000000 0.533350000000 0.071860000000 F F F
 0.030150000000 0.588540000000 0.002300000000 F F F
 0.418730000000 0.700590000000 0.070570000000 F F F
 0.974848817036 0.479190574405 0.142348919227 T T T
 0.585890000000 0.700610000000 0.070280000000 F F F
 0.141931318240 0.479101288738 0.142293201944 T T T
 0.029980000000 0.922770000000 0.002560000000 F F F
 0.418980000000 0.866930000000 0.071690000000 F F F
 0.863530000000 0.922730000000 0.003450000000 F F F
 0.918990000000 0.866770000000 0.072200000000 F F F
 0.808872017402 0.811611342133 0.141804097937 T T T
 0.697080000000 0.922670000000 0.003600000000 F F F
 0.752290000000 0.866490000000 0.072540000000 F F F
 0.641890011730 0.811227245603 0.141703687201 T T T
 0.530550000000 0.922650000000 0.003160000000 F F F
 0.585690000000 0.866680000000 0.072310000000 F F F
 0.475555124520 0.811665643284 0.141434878368 T T T
 0.363980000000 0.922700000000 0.001990000000 F F F
 0.196860000000 0.922600000000 0.001880000000 F F F
 0.308927449025 0.811953858858 0.141187704943 T T T
 0.253170000000 0.867290000000 0.070550000000 F F F
 0.142537577719 0.811915749670 0.140539434214 T T T
 0.530260000000 0.756230000000 0.001760000000 F F F
 0.085480000000 0.867120000000 0.070870000000 F F F
 0.976081846777 0.812010000999 0.141371244207 T T T
 0.863890000000 0.756160000000 0.002120000000 F F F
 0.919460000000 0.700540000000 0.071000000000 F F F
 0.809294717670 0.645518101658 0.141012871483 T T T
 0.697280000000 0.756220000000 0.001970000000 F F F
 0.752920000000 0.700390000000 0.070970000000 F F F
 0.642341130485 0.645012984976 0.140315935087 T T T
 0.085800000000 0.533770000000 0.072730000000 F F F
 0.530500000000 0.088930000000 0.003010000000 F F F
 0.697130000000 0.589150000000 0.001710000000 F F F
 0.141738963136 0.312426812515 0.142343839250 T T T
 0.863550000000 0.421960000000 0.002990000000 F F F
 0.308212688914 0.145614613833 0.142146078731 T T T

0.141660206468 0.145602784091 0.142278317714 T T T
 0.029990000000 0.255660000000 0.003890000000 F F F
 0.085720000000 0.200180000000 0.072890000000 F F F
 0.974430610245 0.145405658440 0.142550257840 T T T
 0.863480000000 0.089200000000 0.004000000000 F F F
 0.918890000000 0.033400000000 0.072980000000 F F F
 0.807715589487 0.978420255370 0.142508445773 T T T
 0.697110000000 0.089160000000 0.003920000000 F F F
 0.752250000000 0.033330000000 0.073220000000 F F F
 0.363150000000 0.255160000000 0.002540000000 F F F
 0.418990000000 0.199750000000 0.071750000000 F F F
 0.585870000000 0.033380000000 0.072790000000 F F F
 0.474399816931 0.978628222075 0.142248157945 T T T
 0.363460000000 0.088800000000 0.002680000000 F F F
 0.419220000000 0.033340000000 0.071830000000 F F F
 0.308209496432 0.978435082057 0.141445437365 T T T
 0.196550000000 0.088960000000 0.003040000000 F F F
 0.252140000000 0.033160000000 0.071820000000 F F F
 0.142152818494 0.978524076530 0.141593991713 T T T
 0.029960000000 0.089210000000 0.003620000000 F F F
 0.085570000000 0.033420000000 0.072450000000 F F F
 0.363340000000 0.756020000000 0.001980000000 F F F
 0.640883379099 0.978474445200 0.142499392490 T T T
 0.252380000000 0.199980000000 0.072280000000 F F F
 0.196520000000 0.255470000000 0.003380000000 F F F
 0.474096872492 0.145253963892 0.141900033981 T T T
 0.807523245903 0.312408974618 0.142447256351 T T T
 0.697020000000 0.422200000000 0.002280000000 F F F
 0.752570000000 0.367040000000 0.072090000000 F F F
 0.640882164037 0.311936782203 0.141669440563 T T T
 0.529920000000 0.421970000000 0.001570000000 F F F
 0.585630000000 0.366780000000 0.071000000000 F F F
 0.475276150151 0.312161184396 0.141158205625 T T T
 0.363000000000 0.421890000000 0.002100000000 F F F
 0.418780000000 0.366430000000 0.071160000000 F F F
 0.308660572756 0.312333708339 0.142028537586 T T T
 0.196500000000 0.422030000000 0.003230000000 F F F
 0.919070000000 0.367050000000 0.073130000000 F F F
 0.252540000000 0.366810000000 0.072360000000 F F F
 0.974453674937 0.312308613716 0.142612994148 T T T
 0.863540000000 0.255670000000 0.004050000000 F F F

0.919000000000 0.200260000000 0.073240000000 F F F
 0.807506626268 0.145446454706 0.142614966222 T T T
 0.697000000000 0.255520000000 0.003250000000 F F F
 0.752320000000 0.200340000000 0.073140000000 F F F
 0.640629692819 0.145459697570 0.142437010947 T T T
 0.530100000000 0.255260000000 0.002420000000 F F F
 0.585620000000 0.199780000000 0.072020000000 F F F
 0.030080000000 0.422160000000 0.003880000000 F F F
 0.085830000000 0.366990000000 0.073000000000 F F F
 0.586449112711 0.572830899788 0.472245641011 T T T
 0.617209303115 0.375386228278 0.466623200997 T T T
 0.554534431365 0.475167510772 0.463432883582 T T T
 0.525035253762 0.225617681016 0.464167035112 T T T
 0.896012622609 0.636470793321 0.459324532002 T T T
 0.493793906590 0.721489167341 0.476695667427 T T T
 0.406904625951 0.679162706133 0.462118104044 T T T
 0.353311255914 0.717755893966 0.467834648530 T T T
 0.472115282164 0.839506024800 0.501702715519 T T T
 0.515107875418 0.596915841851 0.462918338635 T T T
 0.326258810060 0.841541888480 0.494890367727 T T T
 0.039476676304 0.663929213589 0.479699895709 T T T
 0.334191180644 0.872797693773 0.537410678330 T T T
 0.226687839107 0.777251132771 0.487456520057 T T T
 0.176090799277 0.798928920468 0.463054893905 T T T
 0.383479848172 0.797417651419 0.488277908506 T T T
 0.180472880783 0.695525299059 0.507428593754 T T T
 0.363963891200 0.925032941570 0.468906154795 T T T
 0.083607776295 0.743722099638 0.459032005285 T T T
 0.088972229113 0.639289862202 0.503579681263 T T T
 0.526720645843 0.802831876342 0.496124133993 T T T
 0.499176363904 0.587290014579 0.431837572798 T T T
 0.594940823316 0.836104603695 0.507086450991 T T T
 0.054422544116 0.576348775972 0.519291877907 T T T
 0.285890132282 0.683679335719 0.456038538306 T T T
 0.682826786639 0.687699869718 0.453508530086 T T T
 0.751548382452 0.419006814349 0.475440384572 T T T
 0.453723141037 0.554858286416 0.479588982506 T T T
 0.499766131103 0.431765813155 0.482894817850 T T T
 0.688887538028 0.511120133931 0.461472613219 T T T
 0.683313443837 0.305822824203 0.468179052899 T T T
 0.528761409252 0.458866519484 0.433670458787 T T T

0.603293160674 0.585723460696 0.503215625774 T T T
 0.380012418235 0.616792698657 0.446116737157 T T T
 0.315616374208 0.817459536586 0.557656510744 T T T
 0.357797204949 0.907328847325 0.438203982036 T T T
 0.217126841936 0.675033774959 0.526505589962 T T T
 0.904974469463 0.638938787575 0.427808780281 T T T
 0.047516496679 0.764334706850 0.439784303332 T T T
 0.434980075967 0.970039262914 0.474827289330 T T T
 0.330553821688 0.963924397196 0.474097606744 T T T
 0.208217491907 0.860801185437 0.446625027151 T T T
 0.289576130530 0.899908631595 0.542287647090 T T T
 0.402376718417 0.925641925480 0.544260377928 T T T
 0.499871037912 0.902860974215 0.517035544963 T T T
 0.826412139903 0.588220340018 0.466306400202 T T T
 0.910833965789 0.702553366033 0.469859483266 T T T
 0.692390035375 0.368324837331 0.465984541383 T T T
 0.512141610412 0.151909110232 0.463631543552 T T T
 0.535319229541 0.306467734260 0.464512053992 T T T
 0.628507632068 0.458823907117 0.468980296662 T T T
 0.665820794715 0.625356879202 0.449691910519 T T T
 0.551751930743 0.688617210551 0.473423969036 T T T
 0.948537676458 0.605989737720 0.478633017958 T T T

The initial structure of the NEB chain for the model with the curing agent (coverage: 20 %)

Au 6 × 6 supercell (3 layers)

1.0
 17.302800000000 0.000000000000 0.000000000000
 -8.651400000000 14.984664356600 0.000000000000
 0.000000000000 0.000000000000 34.709200000000

Au C H N O

108 28 26 11 3

Selective dynamics

Direct

0.999051757667 0.002382322984 0.137086668071 T T T
 0.000321597439 0.837346324173 0.138725380384 T T T
 0.555560000000 0.611110000000 0.000000000000 F F F
 0.055560000000 0.111110000000 0.000000000000 F F F
 0.171774886022 0.006049303482 0.135552844030 T T T
 0.277780000000 0.055560000000 0.067840000000 F F F
 0.222220000000 0.111110000000 0.000000000000 F F F

0.330914891904 0.003127410789 0.137631678630 T T T
 0.444440000000 0.055560000000 0.067840000000 F F F
 0.388890000000 0.111110000000 0.000000000000 F F F
 0.496625070135 0.998669332405 0.136306950024 T T T
 0.611110000000 0.055560000000 0.067840000000 F F F
 0.555560000000 0.111110000000 0.000000000000 F F F
 0.777780000000 0.055560000000 0.067840000000 F F F
 0.444440000000 0.222220000000 0.067840000000 F F F
 0.722220000000 0.111110000000 0.000000000000 F F F
 0.888890000000 0.444440000000 0.000000000000 F F F
 0.944440000000 0.055560000000 0.067840000000 F F F
 0.888890000000 0.111110000000 0.000000000000 F F F
 0.999440133077 0.165206446021 0.139053355695 T T T
 0.055560000000 0.277780000000 0.000000000000 F F F
 0.277780000000 0.222220000000 0.067840000000 F F F
 0.222220000000 0.277780000000 0.000000000000 F F F
 0.345651047784 0.164899494315 0.170181258446 T T T
 0.111110000000 0.055560000000 0.067840000000 F F F
 0.666949768380 0.995661302638 0.137669411924 T T T
 0.165049974214 0.167080237216 0.136450003637 T T T
 0.832500329830 0.997853257261 0.139164612586 T T T
 0.722220000000 0.277780000000 0.000000000000 F F F
 0.663628259027 0.160080859188 0.137153073925 T T T
 0.777780000000 0.222220000000 0.067840000000 F F F
 0.834365956598 0.161590524348 0.136756291612 T T T
 0.944440000000 0.222220000000 0.067840000000 F F F
 0.111110000000 0.388890000000 0.067840000000 F F F
 0.003313262490 0.330022421196 0.137629990102 T T T
 0.277780000000 0.388890000000 0.067840000000 F F F
 0.055560000000 0.444440000000 0.000000000000 F F F
 0.888890000000 0.277780000000 0.000000000000 F F F
 0.555560000000 0.277780000000 0.000000000000 F F F
 0.944440000000 0.388890000000 0.067840000000 F F F
 0.444440000000 0.388890000000 0.067840000000 F F F
 0.555560000000 0.444440000000 0.000000000000 F F F
 0.166778241067 0.332279428367 0.138823444727 T T T
 0.222220000000 0.444440000000 0.000000000000 F F F
 0.330850015085 0.329609326423 0.136638125940 T T T
 0.111110000000 0.222220000000 0.067840000000 F F F
 0.388890000000 0.444440000000 0.000000000000 F F F
 0.491096211922 0.327012065184 0.136312896995 T T T

0.777780000000 0.388890000000 0.067840000000 F F F
 0.722220000000 0.444440000000 0.000000000000 F F F
 0.489482042299 0.163913452913 0.137509542946 T T T
 0.611110000000 0.222220000000 0.067840000000 F F F
 0.838571988475 0.332094462522 0.137570792641 T T T
 0.944440000000 0.722220000000 0.067840000000 F F F
 0.388890000000 0.277780000000 0.000000000000 F F F
 0.222220000000 0.944440000000 0.000000000000 F F F
 0.055560000000 0.611110000000 0.000000000000 F F F
 0.164080005170 0.495909447679 0.137509719923 T T T
 0.277780000000 0.555560000000 0.067840000000 F F F
 0.444440000000 0.555560000000 0.067840000000 F F F
 0.388890000000 0.611110000000 0.000000000000 F F F
 0.611110000000 0.555560000000 0.067840000000 F F F
 0.662155332772 0.499962087750 0.137034639265 T T T
 0.777780000000 0.555560000000 0.067840000000 F F F
 0.722220000000 0.611110000000 0.000000000000 F F F
 0.837228613502 0.502142338905 0.135315752679 T T T
 0.944440000000 0.555560000000 0.067840000000 F F F
 0.888890000000 0.611110000000 0.000000000000 F F F
 0.001754681927 0.666914911494 0.135953985594 T T T
 0.111110000000 0.722220000000 0.067840000000 F F F
 0.055560000000 0.777780000000 0.000000000000 F F F
 0.165483370171 0.664794346002 0.136619185778 T T T
 0.277780000000 0.722220000000 0.067840000000 F F F
 0.222220000000 0.777780000000 0.000000000000 F F F
 0.332417870441 0.660956834178 0.137944419771 T T T
 0.444440000000 0.722220000000 0.067840000000 F F F
 0.003011546105 0.502334111514 0.137133435818 T T T
 0.611110000000 0.388890000000 0.067840000000 F F F
 0.661775262006 0.329052902768 0.136887096356 T T T
 0.388890000000 0.777780000000 0.000000000000 F F F
 0.500533976851 0.663843654448 0.137823924091 T T T
 0.222220000000 0.611110000000 0.000000000000 F F F
 0.555560000000 0.777780000000 0.000000000000 F F F
 0.662494281324 0.664266702781 0.138372678028 T T T
 0.777780000000 0.722220000000 0.067840000000 F F F
 0.611110000000 0.722220000000 0.067840000000 F F F
 0.828919123494 0.665983422565 0.138728558899 T T T
 0.497474381718 0.496853672567 0.137231506751 T T T
 0.111110000000 0.888890000000 0.067840000000 F F F

0.055560000000 0.944440000000 0.000000000000 F F F
 0.332203613755 0.493744459553 0.138003680057 T T T
 0.277780000000 0.888890000000 0.067840000000 F F F
 0.331718447050 0.834665454419 0.139850105654 T T T
 0.722220000000 0.777780000000 0.000000000000 F F F
 0.888890000000 0.777780000000 0.000000000000 F F F
 0.111110000000 0.555560000000 0.067840000000 F F F
 0.165153346722 0.833379975832 0.136017287153 T T T
 0.388890000000 0.944440000000 0.000000000000 F F F
 0.501797482769 0.833993483605 0.136150010175 T T T
 0.611110000000 0.888890000000 0.067840000000 F F F
 0.944440000000 0.888890000000 0.067840000000 F F F
 0.555560000000 0.944440000000 0.000000000000 F F F
 0.664957416200 0.830554635233 0.138951671674 T T T
 0.777780000000 0.888890000000 0.067840000000 F F F
 0.722220000000 0.944440000000 0.000000000000 F F F
 0.829822397988 0.833252722762 0.136720755036 T T T
 0.444440000000 0.888890000000 0.067840000000 F F F
 0.888890000000 0.944440000000 0.000000000000 F F F
 0.456559068366 0.216736615708 0.240950333250 T T T
 0.365445250884 0.495646203203 0.301321776704 T T T
 0.997803148864 0.621313346440 0.238377598728 T T T
 0.217440847599 0.459974664608 0.281578582479 T T T
 0.116915578349 0.582591491262 0.234111803618 T T T
 0.295483015558 0.397612978728 0.247579971739 T T T
 0.353007673720 0.266691749501 0.284738259185 T T T
 0.386785376808 0.153151638882 0.264368244711 T T T
 0.220208580932 0.405849172183 0.252059128654 T T T
 0.504139977445 0.488420188874 0.231833459096 T T T
 0.143773746830 0.541370683392 0.300505730346 T T T
 0.420582818093 0.038288697027 0.249478701652 T T T
 0.473795474994 0.305147120483 0.240602774195 T T T
 0.369600088603 0.441421472849 0.272413039747 T T T
 0.686094705977 0.397871479490 0.187478700308 T T T
 0.648406005705 0.165322376466 0.194560927461 T T T
 0.334049140757 0.178966696856 0.285611521597 T T T
 0.021695678164 0.859143360825 0.196005987651 T T T
 0.874357713888 0.629828343143 0.216666547543 T T T
 0.451603869548 0.431008926871 0.266931233094 T T T
 0.870894995925 0.353069890843 0.194495253366 T T T
 0.179349369991 0.613334238145 0.269159184446 T T T

0.320589497254 0.824281698975 0.198192575200 TTT
 0.363221432121 0.652927103225 0.193856306070 TTT
 0.424022691247 0.332460311309 0.262539630549 TTT
 0.516262365728 0.466312227362 0.301801854863 TTT
 0.291144519734 0.505753929491 0.305971211205 TTT
 0.240659517689 0.159780242207 0.197653957711 TTT
 0.464794247125 0.461390486497 0.205182831571 TTT
 0.572183515855 0.454546514484 0.296699249466 TTT
 0.516628886392 0.556816200997 0.235290895659 TTT
 0.568621401769 0.491262680187 0.228186610909 TTT
 0.544121623385 0.538513372055 0.305651931310 TTT
 0.039117218985 0.755890928694 0.240238874569 TTT
 0.115472137536 0.723378200963 0.256564766764 TTT
 0.421200964946 0.531180929625 0.321081376017 TTT
 0.491522022088 0.080436794209 0.256740100268 TTT
 0.412529244721 0.039258706327 0.217897597870 TTT
 0.503562008936 0.201192415410 0.226928817522 TTT
 0.482914663788 0.432297628020 0.328645043807 TTT
 0.162388689665 0.370367822377 0.233218878037 TTT
 0.243676789330 0.744230295102 0.271652813093 TTT
 0.295858323877 0.354420110496 0.224749810164 TTT
 0.185516746523 0.566172970948 0.326415024962 TTT
 0.074910726250 0.521572265420 0.308419613857 TTT
 0.244005844754 0.622946742955 0.259043249982 TTT
 0.975826743141 0.495030722837 0.238493055373 TTT
 0.146693791694 0.634444310410 0.211462610044 TTT
 0.395448329468 0.969537554939 0.258826595236 TTT
 0.279287553549 0.128812487958 0.302888157178 TTT
 0.291156175399 0.548733033335 0.328871467053 TTT
 0.113537001509 0.521739818485 0.222685964496 TTT
 0.312298544620 0.285532501988 0.301961747455 TTT
 0.531443115749 0.354008942941 0.224368350089 TTT
 0.909695485070 0.587477364788 0.231038546330 TTT
 0.309729299492 0.814924383671 0.231560871717 TTT
 0.834092902310 0.661853552010 0.201782154769 TTT
 0.057174081230 0.707983391502 0.242412543625 TTT
 0.901543911216 0.375233162211 0.225427838295 TTT
 0.382778158063 0.644801455564 0.225415645479 TTT
 0.037694434829 0.868923199954 0.229099219477 TTT
 0.180586470516 0.159757812284 0.213975748591 TTT
 0.635619189224 0.167072213812 0.227675573473 TTT

```

0.693243415910 0.435866705717 0.216637143942 TTT
0.025212360962 0.561215860663 0.240790996344 TTT
0.191353858426 0.695037283827 0.285020827031 TTT
0.366345233140 0.067434206876 0.268719011529 TTT
0.139448314382 0.462041711325 0.285165594504 TTT

```

The final structure of the NEB chain for the model with the curing agent (coverage: 20 %)

Au 6 × 6 supercell (3 layers)

```

1.0
17.302800000000 0.000000000000 0.000000000000
-8.651400000000 14.984664356600 0.000000000000
0.000000000000 0.000000000000 34.709200000000

```

Au C H N O

108 28 26 11 3

Selective dynamics

Direct

```

0.999289467214 0.001558295586 0.136893753337 TTT
-0.001118650752 0.833834658104 0.139786856156 TTT
0.555560000000 0.611110000000 0.000000000000 FFF
0.055560000000 0.111110000000 0.000000000000 FFF
0.169305541862 0.003410145480 0.135387871367 TTT
0.277780000000 0.055560000000 0.067840000000 FFF
0.222220000000 0.111110000000 0.000000000000 FFF
0.330682463760 0.001635505436 0.137169067853 TTT
0.444440000000 0.055560000000 0.067840000000 FFF
0.388890000000 0.111110000000 0.000000000000 FFF
0.497685013688 0.998694807752 0.136616233844 TTT
0.611110000000 0.055560000000 0.067840000000 FFF
0.555560000000 0.111110000000 0.000000000000 FFF
0.777780000000 0.055560000000 0.067840000000 FFF
0.444440000000 0.222220000000 0.067840000000 FFF
0.722220000000 0.111110000000 0.000000000000 FFF
0.888890000000 0.444440000000 0.000000000000 FFF
0.944440000000 0.055560000000 0.067840000000 FFF
0.888890000000 0.111110000000 0.000000000000 FFF
0.999438447989 0.165426733353 0.138669616421 TTT
0.055560000000 0.277780000000 0.000000000000 FFF
0.277780000000 0.222220000000 0.067840000000 FFF
0.222220000000 0.277780000000 0.000000000000 FFF
0.348436922600 0.161580411993 0.168531194581 TTT

```

0.111110000000 0.055560000000 0.067840000000 F F F
 0.668102884241 0.996590400332 0.137730331122 T T T
 0.165233940647 0.167150129420 0.136570641499 T T T
 0.833521374346 0.998153314659 0.139137707195 T T T
 0.722220000000 0.277780000000 0.000000000000 F F F
 0.666598522186 0.161601345791 0.136766617216 T T T
 0.777780000000 0.222220000000 0.067840000000 F F F
 0.834718107491 0.162247892050 0.136969141104 T T T
 0.944440000000 0.222220000000 0.067840000000 F F F
 0.111110000000 0.388890000000 0.067840000000 F F F
 0.003212172353 0.330713492945 0.137442733864 T T T
 0.277780000000 0.388890000000 0.067840000000 F F F
 0.055560000000 0.444440000000 0.000000000000 F F F
 0.888890000000 0.277780000000 0.000000000000 F F F
 0.555560000000 0.277780000000 0.000000000000 F F F
 0.944440000000 0.388890000000 0.067840000000 F F F
 0.444440000000 0.388890000000 0.067840000000 F F F
 0.555560000000 0.444440000000 0.000000000000 F F F
 0.167051132908 0.332949333529 0.138605795027 T T T
 0.222220000000 0.444440000000 0.000000000000 F F F
 0.331849267706 0.331326555931 0.136288935597 T T T
 0.111110000000 0.222220000000 0.067840000000 F F F
 0.388890000000 0.444440000000 0.000000000000 F F F
 0.490659083047 0.326613936753 0.136154292812 T T T
 0.777780000000 0.388890000000 0.067840000000 F F F
 0.722220000000 0.444440000000 0.000000000000 F F F
 0.491818804438 0.163135490832 0.137035242560 T T T
 0.611110000000 0.222220000000 0.067840000000 F F F
 0.838607128080 0.334288773009 0.137239400396 T T T
 0.944440000000 0.722220000000 0.067840000000 F F F
 0.388890000000 0.277780000000 0.000000000000 F F F
 0.222220000000 0.944440000000 0.000000000000 F F F
 0.055560000000 0.611110000000 0.000000000000 F F F
 0.164913976925 0.497252643914 0.137388830013 T T T
 0.277780000000 0.555560000000 0.067840000000 F F F
 0.444440000000 0.555560000000 0.067840000000 F F F
 0.388890000000 0.611110000000 0.000000000000 F F F
 0.611110000000 0.555560000000 0.067840000000 F F F
 0.665607761325 0.503634785075 0.137240827967 T T T
 0.777780000000 0.555560000000 0.067840000000 F F F
 0.722220000000 0.611110000000 0.000000000000 F F F

0.838011539205 0.505590671977 0.136426915413 TTT
 0.944440000000 0.555560000000 0.067840000000 FFF
 0.888890000000 0.611110000000 0.000000000000 FFF
 0.001052014144 0.667000957240 0.137565155864 TTT
 0.111110000000 0.722220000000 0.067840000000 FFF
 0.055560000000 0.777780000000 0.000000000000 FFF
 0.165439387599 0.664447282116 0.136741467676 TTT
 0.277780000000 0.722220000000 0.067840000000 FFF
 0.222220000000 0.777780000000 0.000000000000 FFF
 0.330819374245 0.661724508485 0.138008908798 TTT
 0.444440000000 0.722220000000 0.067840000000 FFF
 0.003129390660 0.503017607795 0.138072442901 TTT
 0.611110000000 0.388890000000 0.067840000000 FFF
 0.661473223837 0.328589844457 0.137036414264 TTT
 0.388890000000 0.777780000000 0.000000000000 FFF
 0.503530544530 0.664991096708 0.137422922624 TTT
 0.222220000000 0.611110000000 0.000000000000 FFF
 0.555560000000 0.777780000000 0.000000000000 FFF
 0.666424912836 0.666455111171 0.138708449376 TTT
 0.777780000000 0.722220000000 0.067840000000 FFF
 0.611110000000 0.722220000000 0.067840000000 FFF
 0.832071225427 0.667509023812 0.136931812591 TTT
 0.499006020730 0.497477734227 0.138139029880 TTT
 0.111110000000 0.888890000000 0.067840000000 FFF
 0.055560000000 0.944440000000 0.000000000000 FFF
 0.332535549076 0.494887102989 0.137265284948 TTT
 0.277780000000 0.888890000000 0.067840000000 FFF
 0.332052138867 0.834332187463 0.139063983528 TTT
 0.722220000000 0.777780000000 0.000000000000 FFF
 0.888890000000 0.777780000000 0.000000000000 FFF
 0.111110000000 0.555560000000 0.067840000000 FFF
 0.165183603038 0.832802322060 0.136064818223 TTT
 0.388890000000 0.944440000000 0.000000000000 FFF
 0.503163838757 0.835643324042 0.135997000324 TTT
 0.611110000000 0.888890000000 0.067840000000 FFF
 0.944440000000 0.888890000000 0.067840000000 FFF
 0.555560000000 0.944440000000 0.000000000000 FFF
 0.667254167810 0.832374148306 0.138514643980 TTT
 0.777780000000 0.888890000000 0.067840000000 FFF
 0.722220000000 0.944440000000 0.000000000000 FFF
 0.831020293252 0.832543980951 0.136838276218 TTT

0.444440000000 0.888890000000 0.067840000000 F F F
 0.888890000000 0.944440000000 0.000000000000 F F F
 0.459973793200 0.229853453312 0.425488426729 T T T
 0.377488734183 0.515467495386 0.481719739822 T T T
 0.955505741850 0.571202097301 0.430201709198 T T T
 0.227952807698 0.467131405735 0.459032560371 T T T
 0.107452620752 0.591276633023 0.415887829139 T T T
 0.312899803944 0.403314960213 0.432599770851 T T T
 0.389583519835 0.294130751774 0.480982857954 T T T
 0.402165980157 0.172229609844 0.453893215014 T T T
 0.235078618642 0.407717492374 0.433740326681 T T T
 0.521726540660 0.502875240561 0.416821244171 T T T
 0.136717428718 0.530993097102 0.478132605699 T T T
 0.405944446791 0.045319553991 0.428265766544 T T T
 0.482009908621 0.319240463259 0.425258849980 T T T
 0.386064153687 0.456670178204 0.456760130896 T T T
 0.683253920809 0.404608888738 0.185551621914 T T T
 0.633854653134 0.164699867307 0.192267139606 T T T
 0.367213428773 0.205363759007 0.481860013332 T T T
 0.019270995418 0.853876007688 0.197024372282 T T T
 0.810365277575 0.537686851048 0.435540352757 T T T
 0.471883594929 0.451582614657 0.453585097818 T T T
 0.873724241744 0.352956008909 0.193670626992 T T T
 0.165014679788 0.612833461040 0.452327071528 T T T
 0.321601556095 0.832225346520 0.197050559527 T T T
 0.404819096824 0.677105969913 0.186854637747 T T T
 0.447504068070 0.353514818976 0.452633763091 T T T
 0.535729602847 0.495889490452 0.488139677015 T T T
 0.300069896248 0.521748255015 0.482918923538 T T T
 0.251039675777 0.165715053145 0.197823999901 T T T
 0.482915852158 0.471724859071 0.390603751709 T T T
 0.594903878057 0.488819251213 0.484605584660 T T T
 0.533060870216 0.571230009477 0.418270747769 T T T
 0.587450043496 0.507835490805 0.414605111600 T T T
 0.559686718290 0.567895189887 0.489384883977 T T T
 -0.052576921888 0.677884768811 0.448780118428 T T T
 0.052617957198 0.688646501126 0.454071317231 T T T
 0.432111295790 0.558087458785 0.500986277321 T T T
 0.479179964197 0.076609537621 0.428694282534 T T T
 0.383765385434 0.051276711664 0.399211583452 T T T
 0.488291138478 0.206315459277 0.403554252927 T T T

0.503834804690 0.465833152274 0.515761044364 TTT
 0.178550876952 0.365370096167 0.415249464444 TTT
 0.197949661575 0.701310280991 0.494861114998 TTT
 0.316958407095 0.356526131626 0.412721078895 TTT
 0.173814602257 0.550611889726 0.505541719315 TTT
 0.065333454363 0.500283361715 0.484818050827 TTT
 0.234823630339 0.639958455972 0.442840962198 TTT
 0.978679144737 0.475279054287 0.412808225336 TTT
 0.125114185939 0.654361438485 0.401097112139 TTT
 0.375591969843 0.974658706781 0.435872273697 TTT
 0.322695703314 0.159757409022 0.503794268455 TTT
 0.297199613790 0.568910928365 0.502771416260 TTT
 0.125281821239 0.552633223499 0.396393902824 TTT
 0.361273671804 0.318581244059 0.502656279745 TTT
 0.527448579690 0.362798107030 0.403069554390 TTT
 0.869132218760 0.514515004915 0.425443370780 TTT
 0.312958681113 0.831179410953 0.230612970493 TTT
 0.753332281265 0.553145336547 0.444006218437 TTT
 -0.008928202943 0.657255255271 0.441602696442 TTT
 0.902337126573 0.366827555038 0.225197080357 TTT
 0.441782827912 0.681652319874 0.216076090592 TTT
 0.033240174521 0.868598829969 0.230070397971 TTT
 0.188812411391 0.168017839254 0.210688232938 TTT
 0.608853374391 0.163237826458 0.223894215492 TTT
 0.691474661977 0.449119010208 0.212796609254 TTT
 0.011608339664 0.539375389859 0.422137692659 TTT
 0.156132139039 0.679698254186 0.473455887267 TTT
 0.375697347603 0.083825123538 0.456905590628 TTT
 0.146616629772 0.463609815158 0.458728898505 TTT

The initial structure of the NEB chain for the model with the curing agent (coverage: 33 %)

Au 6 × 6 supercell (3 layers)

1.0

17.302800000000 0.000000000000 0.000000000000
 -8.651400000000 14.984664356600 0.000000000000
 0.000000000000 0.000000000000 34.709200000000

Au C H N O

108 33 26 16 3

Selective dynamics

Direct

0.002062531007 0.004303491681 0.164637811080 TTT
 0.555560000000 0.611110000000 0.028810000000 FFF
 0.055560000000 0.111110000000 0.028810000000 FFF
 0.170176040846 0.000697015271 0.166637480122 TTT
 0.277780000000 0.055560000000 0.096650000000 FFF
 0.222220000000 0.111110000000 0.028810000000 FFF
 0.336905536233 0.005604360550 0.166996234487 TTT
 0.444440000000 0.055560000000 0.096650000000 FFF
 0.388890000000 0.111110000000 0.028810000000 FFF
 0.502831272829 0.003241993778 0.166085084631 TTT
 0.611110000000 0.055560000000 0.096650000000 FFF
 0.555560000000 0.111110000000 0.028810000000 FFF
 0.777780000000 0.055560000000 0.096650000000 FFF
 0.444440000000 0.222220000000 0.096650000000 FFF
 0.722220000000 0.111110000000 0.028810000000 FFF
 0.888890000000 0.444440000000 0.028810000000 FFF
 0.944440000000 0.055560000000 0.096650000000 FFF
 0.888890000000 0.111110000000 0.028810000000 FFF
 0.000741749084 0.167680054538 0.166235664631 TTT
 0.055560000000 0.277780000000 0.028810000000 FFF
 0.166990071040 0.168215543975 0.167003143670 TTT
 0.277780000000 0.222220000000 0.096650000000 FFF
 0.222220000000 0.277780000000 0.028810000000 FFF
 0.336739411729 0.169430543830 0.164017292916 TTT
 0.111110000000 0.055560000000 0.096650000000 FFF
 0.666207518836 0.001043192836 0.166465277147 TTT
 0.111110000000 0.222220000000 0.096650000000 FFF
 0.837861999166 0.001521996483 0.164729367213 TTT
 0.277780000000 0.388890000000 0.096650000000 FFF
 0.777780000000 0.222220000000 0.096650000000 FFF
 0.834540087339 0.168224524376 0.165926461011 TTT
 0.944440000000 0.222220000000 0.096650000000 FFF
 0.111110000000 0.388890000000 0.096650000000 FFF
 0.722220000000 0.277780000000 0.028810000000 FFF
 0.996017007165 0.329193002030 0.165042770749 TTT
 0.055560000000 0.444440000000 0.028810000000 FFF
 0.888890000000 0.277780000000 0.028810000000 FFF
 0.555560000000 0.277780000000 0.028810000000 FFF
 0.666261727150 0.173451958941 0.166584725440 TTT
 0.830641288293 0.337063487862 0.167375866979 TTT
 0.611110000000 0.388890000000 0.096650000000 FFF

0.164817964235 0.334365718397 0.167259706294 TTT
 0.222220000000 0.444440000000 0.028810000000 FFF
 0.388890000000 0.444440000000 0.028810000000 FFF
 0.513093479132 0.349574318094 0.193552528723 TTT
 0.388890000000 0.277780000000 0.028810000000 FFF
 0.555560000000 0.444440000000 0.028810000000 FFF
 0.665691558489 0.338780951379 0.165687510807 TTT
 0.777780000000 0.388890000000 0.096650000000 FFF
 0.722220000000 0.444440000000 0.028810000000 FFF
 0.500507100403 0.173927069887 0.163359850816 TTT
 0.611110000000 0.222220000000 0.096650000000 FFF
 0.944440000000 0.388890000000 0.096650000000 FFF
 0.166588319318 0.831707942914 0.164174455621 TTT
 0.343222167324 0.337943209155 0.164968567116 TTT
 0.826316087218 0.665514368561 0.164229278735 TTT
 0.055560000000 0.611110000000 0.028810000000 FFF
 0.173030884169 0.502992793418 0.166182434782 TTT
 0.277780000000 0.555560000000 0.096650000000 FFF
 0.222220000000 0.611110000000 0.028810000000 FFF
 0.338753789057 0.500761944128 0.164957924527 TTT
 0.388890000000 0.611110000000 0.028810000000 FFF
 0.501581602882 0.498799782329 0.166698443757 TTT
 0.611110000000 0.555560000000 0.096650000000 FFF
 0.661185106084 0.497739432582 0.166535989770 TTT
 0.777780000000 0.555560000000 0.096650000000 FFF
 0.722220000000 0.611110000000 0.028810000000 FFF
 0.826242804721 0.500579246107 0.166679679493 TTT
 0.944440000000 0.555560000000 0.096650000000 FFF
 0.888890000000 0.611110000000 0.028810000000 FFF
 0.000899354368 0.665772895729 0.165964229756 TTT
 0.111110000000 0.722220000000 0.096650000000 FFF
 0.055560000000 0.777780000000 0.028810000000 FFF
 0.171386840741 0.665981692504 0.167726735018 TTT
 0.222220000000 0.777780000000 0.028810000000 FFF
 0.336909927335 0.665950143847 0.166219861258 TTT
 0.444440000000 0.722220000000 0.096650000000 FFF
 0.002337469324 0.499152222232 0.165157340264 TTT
 0.444440000000 0.388890000000 0.096650000000 FFF
 0.388890000000 0.777780000000 0.028810000000 FFF
 0.499773846573 0.663074776016 0.166731744415 TTT
 0.444440000000 0.555560000000 0.096650000000 FFF

0.555560000000 0.777780000000 0.028810000000 F F F
 0.662687409243 0.661812161894 0.165495464223 T T T
 0.611110000000 0.722220000000 0.096650000000 F F F
 0.777780000000 0.722220000000 0.096650000000 F F F
 0.722220000000 0.777780000000 0.028810000000 F F F
 0.944440000000 0.722220000000 0.096650000000 F F F
 0.888890000000 0.777780000000 0.028810000000 F F F
 0.277780000000 0.722220000000 0.096650000000 F F F
 0.111110000000 0.888890000000 0.096650000000 F F F
 0.055560000000 0.944440000000 0.028810000000 F F F
 0.277780000000 0.888890000000 0.096650000000 F F F
 0.332202716914 0.830092695400 0.164713763777 T T T
 0.444440000000 0.888890000000 0.096650000000 F F F
 0.222220000000 0.944440000000 0.028810000000 F F F
 0.003207975955 0.834304622217 0.166070279415 T T T
 0.888890000000 0.944440000000 0.028810000000 F F F
 0.111110000000 0.555560000000 0.096650000000 F F F
 0.388890000000 0.944440000000 0.028810000000 F F F
 0.500057268826 0.831184790839 0.165963381347 T T T
 0.555560000000 0.944440000000 0.028810000000 F F F
 0.944440000000 0.888890000000 0.096650000000 F F F
 0.611110000000 0.888890000000 0.096650000000 F F F
 0.777780000000 0.888890000000 0.096650000000 F F F
 0.722220000000 0.944440000000 0.028810000000 F F F
 0.833977248427 0.834848178796 0.168845891354 T T T
 0.664706504547 0.829049999212 0.166324108516 T T T
 0.589068261513 0.326656962397 0.299322752646 T T T
 0.518744057166 0.288989957310 0.326407533375 T T T
 0.526834861932 0.431656569410 0.333813949713 T T T
 0.487624047267 0.342637384906 0.343420234586 T T T
 0.641587474537 0.571476777043 0.299056801230 T T T
 0.702101760560 0.621439098139 0.333925171923 T T T
 0.266782972595 0.778177001149 0.319619402615 T T T
 0.336685780399 0.762231699196 0.299409846358 T T T
 0.211824881076 0.872943510977 0.288959105569 T T T
 0.500658455621 0.141719045087 0.321426559905 T T T
 0.561549506456 0.660394092215 0.313703372874 T T T
 0.490936175897 0.676406835931 0.308812480318 T T T
 0.627089960193 0.416528160920 0.289914046550 T T T
 0.597866469906 0.471368783827 0.306947376064 T T T
 0.702304156000 0.600880511461 0.263134780566 T T T

0.423333813239 0.625302106798 0.282114134931 TTT
 0.498386352120 0.543018287489 0.266392145933 TTT
 0.427898988026 0.558417579709 0.260816051559 TTT
 0.747873957381 0.826602050768 0.214503167211 TTT
 0.313680095318 0.664600865040 0.304386333671 TTT
 0.202236728376 0.979997211079 0.252676398859 TTT
 0.978744318598 0.824514464562 0.223738240797 TTT
 0.234662721394 0.238110421875 0.215188799010 TTT
 0.940518150434 0.392103937072 0.209838806656 TTT
 0.147064928852 0.647446283283 0.224806746026 TTT
 0.567145804576 0.593517878954 0.293011384805 TTT
 0.171223919909 0.410749870958 0.215041014802 TTT
 0.438877526279 0.236623963660 0.223423670753 TTT
 0.761912227923 0.049706943873 0.211131687913 TTT
 0.408977088832 0.990203904216 0.213279866695 TTT
 0.521881459394 0.849387874005 0.223109170056 TTT
 0.926457000209 0.603828722786 0.214599281281 TTT
 0.665335340587 0.187830756833 0.224209490353 TTT
 0.116848809858 0.740237710670 0.281616875583 TTT
 0.498092015075 0.487875682945 0.250919224055 TTT
 0.079781318728 0.815988500354 0.273157681615 TTT
 0.337149773625 0.915511160747 0.304995575533 TTT
 0.737874228083 0.693858156065 0.328957914908 TTT
 0.241511540939 0.619959444634 0.300796791920 TTT
 0.335056013332 0.774148961786 0.268179175807 TTT
 0.334595951977 0.654443741465 0.332948874036 TTT
 0.489057538021 0.729552259007 0.324876696024 TTT
 0.199400532912 0.722804611439 0.314210134004 TTT
 0.279342799686 0.782363725302 0.350878648768 TTT
 0.371868931997 0.515530474932 0.242179770159 TTT
 0.477999347593 0.128422274957 0.291374848329 TTT
 0.613802490361 0.701883245674 0.334091074854 TTT
 0.464451611702 0.080731897479 0.338513459660 TTT
 0.572736760777 0.166907298031 0.322919552503 TTT
 0.502212251538 0.472365361866 0.347095050934 TTT
 0.467846261417 0.844229753034 0.295644284386 TTT
 0.432687534245 0.311868184559 0.363918354073 TTT
 0.614014672003 0.286306063699 0.285957753667 TTT
 0.663989517559 0.606761946864 0.360856541364 TTT
 0.759249900863 0.590124854946 0.266736633055 TTT
 0.728446137013 0.672216059436 0.258065104525 TTT

0.751995557091 0.600484091591 0.337429944241 TTT
 0.681936300905 0.444581124256 0.269281883854 TTT
 0.664784347573 0.564006223110 0.237408254190 TTT
 0.175916096639 0.436328424413 0.246988330954 TTT
 0.534868900722 0.861545552437 0.256252328045 TTT
 0.732569156764 0.818872884198 0.247947257525 TTT
 0.273279976272 0.281758372692 0.242263191138 TTT
 0.129188519458 0.638439479584 0.257684968570 TTT
 0.946593482391 0.388823888316 0.243785142981 TTT
 0.890362706029 0.575854058611 0.244445881863 TTT
 0.417253584253 0.981675531465 0.246576281611 TTT
 0.970398513917 0.818218369543 0.257332776921 TTT
 0.130330657023 0.804850874580 0.281282115950 TTT
 0.794123813613 0.062370745256 0.242273346210 TTT
 0.237266880948 0.958906181054 0.279760051515 TTT
 0.274351358115 0.861588826434 0.306580134954 TTT
 0.666039811988 0.202305209729 0.257244431245 TTT
 0.397714513251 0.174968698584 0.244030235979 TTT
 0.173004402011 0.006866441969 0.228119280233 TTT
 0.420346067603 0.824571628832 0.315636794711 TTT
 0.477571719720 0.203714211832 0.338387803438 TTT
 0.352107597839 0.635752394223 0.274616857014 TTT

The final structure of the NEB chain for the model with the curing agent (coverage: 33 %)

Au 6 × 6 supercell (3 layers)

1.0
 17.302800000000 0.000000000000 0.000000000000
 -8.651400000000 14.984664356600 0.000000000000
 0.000000000000 0.000000000000 34.709200000000

Au C H N O

108 33 26 16 3

Selective dynamics

Direct

0.002018419345 0.002826609016 0.165338499048 TTT
 0.555560000000 0.611110000000 0.028810000000 FFF
 0.055560000000 0.111110000000 0.028810000000 FFF
 0.167362633035 -0.000610052939 0.166307450477 TTT
 0.277780000000 0.055560000000 0.096650000000 FFF
 0.222220000000 0.111110000000 0.028810000000 FFF
 0.334511464260 0.007134021403 0.166532213719 TTT

0.444440000000 0.055560000000 0.096650000000 F F F
 0.388890000000 0.111110000000 0.028810000000 F F F
 0.504279979657 0.005747597316 0.166822950519 T T T
 0.611110000000 0.055560000000 0.096650000000 F F F
 0.555560000000 0.111110000000 0.028810000000 F F F
 0.777780000000 0.055560000000 0.096650000000 F F F
 0.444440000000 0.222220000000 0.096650000000 F F F
 0.722220000000 0.111110000000 0.028810000000 F F F
 0.888890000000 0.444440000000 0.028810000000 F F F
 0.944440000000 0.055560000000 0.096650000000 F F F
 0.888890000000 0.111110000000 0.028810000000 F F F
 -0.000134623240 0.165654989627 0.166210846296 T T T
 0.055560000000 0.277780000000 0.028810000000 F F F
 0.164957362932 0.163694612308 0.167739033571 T T T
 0.277780000000 0.222220000000 0.096650000000 F F F
 0.222220000000 0.277780000000 0.028810000000 F F F
 0.331992571696 0.163778584796 0.164076360813 T T T
 0.111110000000 0.055560000000 0.096650000000 F F F
 0.665380752918 -0.000353270717 0.166876307435 T T T
 0.111110000000 0.222220000000 0.096650000000 F F F
 0.837268386085 0.000488596406 0.164881212418 T T T
 0.277780000000 0.388890000000 0.096650000000 F F F
 0.777780000000 0.222220000000 0.096650000000 F F F
 0.834525191982 0.167640637143 0.166233784025 T T T
 0.944440000000 0.222220000000 0.096650000000 F F F
 0.111110000000 0.388890000000 0.096650000000 F F F
 0.722220000000 0.277780000000 0.028810000000 F F F
 0.996944192701 0.328438513993 0.164847564917 T T T
 0.055560000000 0.444440000000 0.028810000000 F F F
 0.888890000000 0.277780000000 0.028810000000 F F F
 0.555560000000 0.277780000000 0.028810000000 F F F
 0.667967687530 0.172884050503 0.165802448135 T T T
 0.831898623078 0.335443054134 0.167469138877 T T T
 0.611110000000 0.388890000000 0.096650000000 F F F
 0.164200197701 0.331680387572 0.165989684384 T T T
 0.222220000000 0.444440000000 0.028810000000 F F F
 0.388890000000 0.444440000000 0.028810000000 F F F
 0.522612176481 0.356654180517 0.198482890935 T T T
 0.388890000000 0.277780000000 0.028810000000 F F F
 0.555560000000 0.444440000000 0.028810000000 F F F
 0.665430471251 0.338110659381 0.165362050755 T T T

0.777780000000 0.388890000000 0.096650000000 F F F
 0.722220000000 0.444440000000 0.028810000000 F F F
 0.500062623042 0.173296689446 0.163162993312 T T T
 0.611110000000 0.222220000000 0.096650000000 F F F
 0.944440000000 0.388890000000 0.096650000000 F F F
 0.168415285450 0.834033236182 0.164511436782 T T T
 0.346860220839 0.337187546443 0.164523344638 T T T
 0.830148968445 0.666641575950 0.163806186422 T T T
 0.055560000000 0.611110000000 0.028810000000 F F F
 0.173629343016 0.502293688707 0.166774634578 T T T
 0.277780000000 0.555560000000 0.096650000000 F F F
 0.222220000000 0.611110000000 0.028810000000 F F F
 0.340792755319 0.500033816706 0.165763980768 T T T
 0.388890000000 0.611110000000 0.028810000000 F F F
 0.504020338413 0.499719989919 0.168439688577 T T T
 0.611110000000 0.555560000000 0.096650000000 F F F
 0.664329303197 0.499834059399 0.166659727226 T T T
 0.777780000000 0.555560000000 0.096650000000 F F F
 0.722220000000 0.611110000000 0.028810000000 F F F
 0.827662412989 0.498828254399 0.165748954240 T T T
 0.944440000000 0.555560000000 0.096650000000 F F F
 0.888890000000 0.611110000000 0.028810000000 F F F
 0.003720534010 0.667250841269 0.166244162830 T T T
 0.111110000000 0.722220000000 0.096650000000 F F F
 0.055560000000 0.777780000000 0.028810000000 F F F
 0.172235501304 0.666206357193 0.167344820754 T T T
 0.222220000000 0.777780000000 0.028810000000 F F F
 0.337852548305 0.665568654327 0.165533209481 T T T
 0.444440000000 0.722220000000 0.096650000000 F F F
 0.003766545877 0.499734071209 0.165643245932 T T T
 0.444440000000 0.388890000000 0.096650000000 F F F
 0.388890000000 0.777780000000 0.028810000000 F F F
 0.501096413537 0.662426349475 0.166202359191 T T T
 0.444440000000 0.555560000000 0.096650000000 F F F
 0.555560000000 0.777780000000 0.028810000000 F F F
 0.665352860879 0.662894414095 0.166347090205 T T T
 0.611110000000 0.722220000000 0.096650000000 F F F
 0.777780000000 0.722220000000 0.096650000000 F F F
 0.722220000000 0.777780000000 0.028810000000 F F F
 0.944440000000 0.722220000000 0.096650000000 F F F
 0.888890000000 0.777780000000 0.028810000000 F F F

0.277780000000 0.722220000000 0.096650000000 F F F
 0.111110000000 0.888890000000 0.096650000000 F F F
 0.055560000000 0.944440000000 0.028810000000 F F F
 0.277780000000 0.888890000000 0.096650000000 F F F
 0.333173635638 0.831035679599 0.165363214428 T T T
 0.444440000000 0.888890000000 0.096650000000 F F F
 0.222220000000 0.944440000000 0.028810000000 F F F
 0.008123829683 0.835828175588 0.166570876189 T T T
 0.888890000000 0.944440000000 0.028810000000 F F F
 0.111110000000 0.555560000000 0.096650000000 F F F
 0.388890000000 0.944440000000 0.028810000000 F F F
 0.500728247511 0.830661272949 0.166167607022 T T T
 0.555560000000 0.944440000000 0.028810000000 F F F
 0.944440000000 0.888890000000 0.096650000000 F F F
 0.611110000000 0.888890000000 0.096650000000 F F F
 0.777780000000 0.888890000000 0.096650000000 F F F
 0.722220000000 0.944440000000 0.028810000000 F F F
 0.837619765598 0.835605261819 0.168926953432 T T T
 0.665852321001 0.829748394190 0.166143507690 T T T
 0.583423683226 0.323825522769 0.530380670392 T T T
 0.519606432287 0.288221626036 0.559934465423 T T T
 0.537333708435 0.434283066271 0.570798373046 T T T
 0.496974712128 0.344667472013 0.580172469866 T T T
 0.645502052628 0.572210776671 0.532751908945 T T T
 0.706837707860 0.623542585672 0.567043558129 T T T
 0.272470029361 0.778738553077 0.552120815704 T T T
 0.326946114861 0.753797932367 0.525199720542 T T T
 0.230002458819 0.885309705309 0.522336549502 T T T
 0.492780844995 0.138981708660 0.551116248801 T T T
 0.558828507995 0.653694998981 0.549793568367 T T T
 0.487948500285 0.669568765055 0.544068013544 T T T
 0.623646265860 0.414612278320 0.521531448275 T T T
 0.602075236363 0.471927273584 0.541311923947 T T T
 0.703927234780 0.600506137897 0.496080759267 T T T
 0.425776897188 0.623702481303 0.514835894971 T T T
 0.506743542978 0.548677488755 0.497542986017 T T T
 0.436202010896 0.563590043767 0.491247133890 T T T
 0.749788644948 0.812966248078 0.214318700554 T T T
 0.313662823340 0.661841943483 0.534907518463 T T T
 0.207265611736 0.993105520157 0.497131969679 T T T
 0.993429714768 0.842437161738 0.224256702203 T T T

0.235231139597 0.242018742821 0.213396707631 TTT
 0.942128707030 0.394978574131 0.209950071909 TTT
 0.160436776846 0.660444836670 0.225037692525 TTT
 0.569925852419 0.593140566351 0.526991868544 TTT
 0.178574435823 0.416151153798 0.213005532445 TTT
 0.440194341373 0.240625797948 0.223891019739 TTT
 0.761328919570 0.045872629760 0.211213899471 TTT
 0.408069420271 0.965950918928 0.210696148490 TTT
 0.518123349133 0.836388350882 0.223674824297 TTT
 0.926936791192 0.606197970375 0.214094279128 TTT
 0.651455679061 0.188275198336 0.222193731380 TTT
 0.137334160258 0.755352942187 0.506870606525 TTT
 0.512247836275 0.499953249946 0.479548609356 TTT
 0.114713640498 0.837189559953 0.492257253590 TTT
 0.345176526852 0.919115020930 0.548230923233 TTT
 0.740805171817 0.696079934577 0.562277341627 TTT
 0.241883272345 0.611764449963 0.534634261404 TTT
 0.305854010955 0.753091318466 0.495055763142 TTT
 0.340352430307 0.662120462338 0.563727962009 TTT
 0.482834231269 0.718709409806 0.561893800626 TTT
 0.201361137283 0.727804804115 0.551319315320 TTT
 0.294857752259 0.779889321249 0.581950835622 TTT
 0.387452057117 0.528496298662 0.468564666677 TTT
 0.471230959056 0.132138024609 0.520860233998 TTT
 0.606254676241 0.690367975947 0.572704607802 TTT
 0.452326728716 0.075264543000 0.565945070284 TTT
 0.563755509961 0.158153015222 0.552727523214 TTT
 0.517599353151 0.476514200179 0.586343467347 TTT
 0.452983577216 0.821016549572 0.508613012909 TTT
 0.446605288380 0.315919584818 0.602776050198 TTT
 0.601833712797 0.281768147930 0.514020196111 TTT
 0.670193069816 0.608318088467 0.594412013828 TTT
 0.760998285764 0.589591221763 0.499295184231 TTT
 0.730446453101 0.671991747748 0.490855253145 TTT
 0.758250028875 0.604418895114 0.570163861524 TTT
 0.672708508826 0.440313184237 0.498379642454 TTT
 0.666363421229 0.564464083764 0.470318783144 TTT
 0.185130947508 0.432526602011 0.246346494696 TTT
 0.529249718295 0.838924062872 0.257109047477 TTT
 0.719370335648 0.799034509226 0.245781605216 TTT
 0.278316603375 0.290276822467 0.238665522363 TTT

```

0.153610006558 0.657433271386 0.258722671763 TTT
0.948536442590 0.386368065028 0.243533998388 TTT
0.879924093578 0.569630540518 0.240689674194 TTT
0.378060606888 0.947202384751 0.242275481556 TTT
0.988912333371 0.849577633070 0.257690151623 TTT
0.149439170601 0.818548046026 0.509928279414 TTT
0.794400445626 0.060037025749 0.242226186849 TTT
0.258872024521 0.971191140395 0.516684231235 TTT
0.283744562461 0.865532045475 0.543658143488 TTT
0.640476306193 0.202558534962 0.254213434513 TTT
0.383741395151 0.168423030319 0.233517364854 TTT
0.163066892681 0.015926759466 0.480101720418 TTT
0.418064275415 0.822977648536 0.530193733657 TTT
0.476107030726 0.201326903605 0.571375133203 TTT
0.353941789865 0.634043708253 0.506060535561 TTT

```

The initial structure of the NEB chain for the model with the curing agent (coverage: 40 %)

Au 6 × 6 supercell (3 layers)

```

1.0
17.302800000000 0.000000000000 0.000000000000
-8.651400000000 14.984664356600 0.000000000000
0.000000000000 0.000000000000 34.709200000000

```

Au C H N O

108 35 26 18 3

Selective dynamics

Direct

```

0.970779765775 0.971989531549 0.136420000000 TTT
0.944440000000 0.888890000000 0.067840000000 FFF
0.323789765775 0.811989531549 0.135780000000 TTT
0.985789765775 0.811539531549 0.136780000000 TTT
0.111110000000 0.055560000000 0.067840000000 FFF
0.555560000000 0.611110000000 0.000000000000 FFF
0.055560000000 0.111110000000 0.000000000000 FFF
0.147689765775 0.975539531549 0.137460000000 TTT
0.277780000000 0.055560000000 0.067840000000 FFF
0.222220000000 0.111110000000 0.000000000000 FFF
0.322489765775 0.987779531549 0.136960000000 TTT
0.444440000000 0.055560000000 0.067840000000 FFF
0.388890000000 0.111110000000 0.000000000000 FFF
0.489249765775 0.981089531549 0.135370000000 TTT

```

0.611110000000 0.055560000000 0.067840000000 F F F
 0.555560000000 0.111110000000 0.000000000000 F F F
 0.444440000000 0.222220000000 0.067840000000 F F F
 0.722220000000 0.111110000000 0.000000000000 F F F
 0.888890000000 0.444440000000 0.000000000000 F F F
 0.055560000000 0.277780000000 0.000000000000 F F F
 0.149819765775 0.141939531549 0.138030000000 T T T
 0.277780000000 0.222220000000 0.067840000000 F F F
 0.222220000000 0.277780000000 0.000000000000 F F F
 0.325499765775 0.152949531549 0.134890000000 T T T
 0.664829765775 0.980169531549 0.135320000000 T T T
 0.111110000000 0.222220000000 0.067840000000 F F F
 0.888890000000 0.111110000000 0.000000000000 F F F
 0.611110000000 0.222220000000 0.067840000000 F F F
 0.944440000000 0.222220000000 0.067840000000 F F F
 0.654869765775 0.148529531549 0.135890000000 T T T
 0.777780000000 0.222220000000 0.067840000000 F F F
 0.987739765775 0.311589531549 0.137190000000 T T T
 0.722220000000 0.277780000000 0.000000000000 F F F
 0.822619765775 0.143749531549 0.134760000000 T T T
 0.277780000000 0.388890000000 0.067840000000 F F F
 0.055560000000 0.444440000000 0.000000000000 F F F
 0.888890000000 0.277780000000 0.000000000000 F F F
 0.555560000000 0.277780000000 0.000000000000 F F F
 0.111110000000 0.388890000000 0.067840000000 F F F
 0.944440000000 0.388890000000 0.067840000000 F F F
 0.944440000000 0.055560000000 0.067840000000 F F F
 0.163079765775 0.313379531549 0.137130000000 T T T
 0.222220000000 0.444440000000 0.000000000000 F F F
 0.331969765775 0.323309531549 0.137260000000 T T T
 0.444440000000 0.388890000000 0.067840000000 F F F
 0.388890000000 0.444440000000 0.000000000000 F F F
 0.987299765775 0.145339531549 0.134210000000 T T T
 0.388890000000 0.277780000000 0.000000000000 F F F
 0.789170000000 0.074730000000 0.208490000000 T T T
 0.777780000000 0.388890000000 0.067840000000 F F F
 0.722220000000 0.444440000000 0.000000000000 F F F
 0.492489765775 0.153629531549 0.136540000000 T T T
 0.819529765775 0.314729531549 0.137180000000 T T T
 0.818309765775 0.642239531549 0.136670000000 T T T
 0.499299765775 0.323239531549 0.150670000000 T T T

0.277780000000 0.888890000000 0.067840000000 F F F
 0.388890000000 0.777780000000 0.000000000000 F F F
 0.055560000000 0.611110000000 0.000000000000 F F F
 0.161819765775 0.485209531549 0.138220000000 T T T
 0.277780000000 0.555560000000 0.067840000000 F F F
 0.222220000000 0.611110000000 0.000000000000 F F F
 0.611110000000 0.555560000000 0.067840000000 F F F
 0.662850000000 0.492940000000 0.168500000000 T T T
 0.777780000000 0.555560000000 0.067840000000 F F F
 0.490549765775 0.647229531549 0.137140000000 T T T
 0.611110000000 0.388890000000 0.067840000000 F F F
 0.944440000000 0.555560000000 0.067840000000 F F F
 0.888890000000 0.611110000000 0.000000000000 F F F
 0.986469765775 0.643269531549 0.137790000000 T T T
 0.111110000000 0.722220000000 0.067840000000 F F F
 0.055560000000 0.777780000000 0.000000000000 F F F
 0.158079765775 0.647599531549 0.135640000000 T T T
 0.277780000000 0.722220000000 0.067840000000 F F F
 0.222220000000 0.777780000000 0.000000000000 F F F
 0.328409765775 0.650849531549 0.137100000000 T T T
 0.444440000000 0.722220000000 0.067840000000 F F F
 0.777780000000 0.055560000000 0.067840000000 F F F
 0.555560000000 0.444440000000 0.000000000000 F F F
 0.650629765775 0.318919531549 0.136550000000 T T T
 0.992569765775 0.480939531549 0.135340000000 T T T
 0.816289765775 0.480379531549 0.135660000000 T T T
 0.388890000000 0.611110000000 0.000000000000 F F F
 0.722220000000 0.611110000000 0.000000000000 F F F
 0.888890000000 0.944440000000 0.000000000000 F F F
 0.555560000000 0.777780000000 0.000000000000 F F F
 0.654049765775 0.643859531549 0.135840000000 T T T
 0.777780000000 0.722220000000 0.067840000000 F F F
 0.611110000000 0.722220000000 0.067840000000 F F F
 0.444440000000 0.555560000000 0.067840000000 F F F
 0.944440000000 0.722220000000 0.067840000000 F F F
 0.888890000000 0.777780000000 0.000000000000 F F F
 0.111110000000 0.888890000000 0.067840000000 F F F
 0.055560000000 0.944440000000 0.000000000000 F F F
 0.154319765775 0.816719531549 0.138820000000 T T T
 0.496819765775 0.484479531549 0.137270000000 T T T
 0.111110000000 0.555560000000 0.067840000000 F F F

0.328269765775 0.484099531549 0.136410000000 TTT
 0.777780000000 0.888890000000 0.067840000000 FFF
 0.388890000000 0.944440000000 0.000000000000 FFF
 0.444440000000 0.888890000000 0.067840000000 FFF
 0.819099765775 0.805499531549 0.135690000000 TTT
 0.722220000000 0.944440000000 0.000000000000 FFF
 0.722220000000 0.777780000000 0.000000000000 FFF
 0.222220000000 0.944440000000 0.000000000000 FFF
 0.492809765775 0.812629531549 0.137510000000 TTT
 0.555560000000 0.944440000000 0.000000000000 FFF
 0.611110000000 0.888890000000 0.067840000000 FFF
 0.663709765775 0.817409531549 0.138230000000 TTT
 0.173040000000 0.518480000000 0.195970000000 TTT
 0.667899531549 0.268509063098 0.282036779182 TTT
 0.751330000000 0.604770000000 0.196890000000 TTT
 0.539029531549 0.319089063098 0.296736779182 TTT
 0.711400000000 0.127790000000 0.209740000000 TTT
 0.971550000000 0.300350000000 0.193610000000 TTT
 0.000620000000 0.653300000000 0.195450000000 TTT
 0.823270000000 0.393250000000 0.187380000000 TTT
 0.155000000000 0.081760000000 0.184760000000 TTT
 0.509930000000 0.954870000000 0.187520000000 TTT
 0.226560000000 0.822770000000 0.187120000000 TTT
 0.369570000000 0.049410000000 0.192010000000 TTT
 0.871550000000 0.028020000000 0.200510000000 TTT
 0.380420000000 0.278080000000 0.181610000000 TTT
 0.176140000000 0.311540000000 0.193850000000 TTT
 0.618239531549 0.353529063098 0.318876779182 TTT
 0.483189531549 0.392079063098 0.344636779182 TTT
 0.589849531549 0.235019063098 0.258736779182 TTT
 0.532639531549 0.470619063098 0.260656779182 TTT
 0.437459531549 0.708079063098 0.256866779182 TTT
 0.669460000000 0.830000000000 0.196250000000 TTT
 0.371799531549 0.382189063098 0.263936779182 TTT
 0.809009531549 0.276339063098 0.292976779182 TTT
 0.511859531549 0.036949063098 0.321666779182 TTT
 0.682169531549 0.329909063098 0.311906779182 TTT
 0.528289531549 0.261649063098 0.265696779182 TTT
 0.455659531549 0.395399063098 0.275286779182 TTT
 0.432349531549 0.891559063098 0.298876779182 TTT
 0.442159531549 0.525729063098 0.232696779182 TTT

0.375039531549 0.731759063098 0.279136779182 TTT
 0.380769531549 0.622869063098 0.233436779182 TTT
 0.526639531549 0.535459063098 0.239376779182 TTT
 0.377969531549 0.247269063098 0.312816779182 TTT
 0.464589531549 0.338259063098 0.306786779182 TTT
 0.364539531549 0.446889063098 0.243206779182 TTT
 0.543519531549 0.458099063098 0.342886779182 TTT
 0.426959531549 0.402779063098 0.350616779182 TTT
 0.489769531549 0.355109063098 0.368986779182 TTT
 0.844699531549 0.247509063098 0.278296779182 TTT
 0.390779531549 0.207619063098 0.333856779182 TTT
 0.580699531549 0.188109063098 0.235886779182 TTT
 0.629439531549 0.399689063098 0.342346779182 TTT
 0.742219531549 0.357649063098 0.329466779182 TTT
 0.468259531549 0.234159063098 0.248066779182 TTT
 0.798349531549 0.256859063098 0.323536779182 TTT
 0.553169531549 0.724429063098 0.271656779182 TTT
 0.326539531549 0.853419063098 0.261386779182 TTT
 0.354109531549 0.208669063098 0.286096779182 TTT
 0.310549531549 0.321689063098 0.271826779182 TTT
 0.385129531549 0.965169063098 0.272486779182 TTT
 0.478399531549 0.813039063098 0.317186779182 TTT
 0.346069531549 0.636619063098 0.210056779182 TTT
 0.331429531549 0.740979063098 0.259006779182 TTT
 0.332039531549 0.676089063098 0.298466779182 TTT
 0.478439531549 0.763219063098 0.237086779182 TTT
 0.324649531549 0.257739063098 0.324236779182 TTT
 0.846759531549 0.349339063098 0.289846779182 TTT
 0.298579531549 0.436309063098 0.236056779182 TTT
 0.586169531549 0.596829063098 0.230656779182 TTT
 0.598779531549 0.481389063098 0.267816779182 TTT
 0.330379531549 0.568689063098 0.251196779182 TTT
 0.179080000000 0.530960000000 0.229330000000 TTT
 0.522930000000 0.933640000000 0.217930000000 TTT
 0.150030000000 0.060590000000 0.217450000000 TTT
 0.395820000000 0.074320000000 0.223340000000 TTT
 0.179860000000 0.298740000000 0.226810000000 TTT
 0.005150000000 0.647920000000 0.228980000000 TTT
 0.261860000000 0.819170000000 0.215580000000 TTT
 0.660440000000 0.819100000000 0.229660000000 TTT
 0.668950000000 0.161290000000 0.201110000000 TTT

```

0.922290000000 0.006170000000 0.189910000000 TTT
0.363170000000 0.258730000000 0.214600000000 TTT
0.819480000000 0.429260000000 0.215560000000 TTT
0.528269531549 0.111579063098 0.327056779182 TTT
0.500519531549 0.957169063098 0.319006779182 TTT
0.947350000000 0.272610000000 0.224820000000 TTT
0.427789531549 0.811619063098 0.301666779182 TTT
0.792590000000 0.664210000000 0.218580000000 TTT
0.371939531549 0.902189063098 0.279126779182 TTT
0.493569531549 0.697289063098 0.283676779182 TTT
0.724289531549 0.239929063098 0.273316779182 TTT
0.438689531549 0.595589063098 0.215506779182 TTT

```

The final structure of the NEB chain for the model with the curing agent (coverage: 40 %)

Au 6 × 6 supercell (3 layers)

1.0

```

17.302800000000 0.000000000000 0.000000000000
-8.651400000000 14.984664356600 0.000000000000
0.000000000000 0.000000000000 34.709200000000

```

Au C H N O

108 35 26 18 3

Selective dynamics

Direct

```

0.970083368413 0.971586483814 0.136540101999 TTT
0.944440000000 0.888890000000 0.067840000000 FFF
0.324896025074 0.810055555673 0.135526318510 TTT
0.984792232701 0.813019689528 0.136963957799 TTT
0.111110000000 0.055560000000 0.067840000000 FFF
0.555560000000 0.611110000000 0.000000000000 FFF
0.055560000000 0.111110000000 0.000000000000 FFF
0.148922694609 0.977534417283 0.137714561764 TTT
0.277780000000 0.055560000000 0.067840000000 FFF
0.222220000000 0.111110000000 0.000000000000 FFF
0.321089714703 0.981464413249 0.136136873471 TTT
0.444440000000 0.055560000000 0.067840000000 FFF
0.388890000000 0.111110000000 0.000000000000 FFF
0.491513853521 0.978891928571 0.136249951774 TTT
0.611110000000 0.055560000000 0.067840000000 FFF
0.555560000000 0.111110000000 0.000000000000 FFF
0.444440000000 0.222220000000 0.067840000000 FFF

```

0.722220000000 0.111110000000 0.000000000000 F F F
 0.888890000000 0.444440000000 0.000000000000 F F F
 0.055560000000 0.277780000000 0.000000000000 F F F
 0.147734369002 0.141224218623 0.138433105938 T T T
 0.277780000000 0.222220000000 0.067840000000 F F F
 0.222220000000 0.277780000000 0.000000000000 F F F
 0.323673667182 0.150240139986 0.136207266470 T T T
 0.666212895795 0.979317758671 0.135636811406 T T T
 0.111110000000 0.222220000000 0.067840000000 F F F
 0.888890000000 0.111110000000 0.000000000000 F F F
 0.611110000000 0.222220000000 0.067840000000 F F F
 0.944440000000 0.222220000000 0.067840000000 F F F
 0.655908714093 0.146530824665 0.136404981093 T T T
 0.777780000000 0.222220000000 0.067840000000 F F F
 0.988175566112 0.312362029021 0.137549742107 T T T
 0.722220000000 0.277780000000 0.000000000000 F F F
 0.822630056533 0.143628793401 0.134814437438 T T T
 0.277780000000 0.388890000000 0.067840000000 F F F
 0.055560000000 0.444440000000 0.000000000000 F F F
 0.888890000000 0.277780000000 0.000000000000 F F F
 0.555560000000 0.277780000000 0.000000000000 F F F
 0.111110000000 0.388890000000 0.067840000000 F F F
 0.944440000000 0.388890000000 0.067840000000 F F F
 0.944440000000 0.055560000000 0.067840000000 F F F
 0.161669456071 0.313011680738 0.137110509709 T T T
 0.222220000000 0.444440000000 0.000000000000 F F F
 0.328733277967 0.318986269620 0.137615020056 T T T
 0.444440000000 0.388890000000 0.067840000000 F F F
 0.388890000000 0.444440000000 0.000000000000 F F F
 0.986892004384 0.145817770766 0.134334481031 T T T
 0.388890000000 0.277780000000 0.000000000000 F F F
 0.789772507385 0.079774377428 0.208765666535 T T T
 0.777780000000 0.388890000000 0.067840000000 F F F
 0.722220000000 0.444440000000 0.000000000000 F F F
 0.494565454910 0.152273704180 0.136621012279 T T T
 0.821867353004 0.315191437666 0.137101298155 T T T
 0.820403784623 0.644435197067 0.135984273181 T T T
 0.500489842296 0.323742809137 0.138324410052 T T T
 0.277780000000 0.888890000000 0.067840000000 F F F
 0.388890000000 0.777780000000 0.000000000000 F F F
 0.055560000000 0.611110000000 0.000000000000 F F F

0.160524886615 0.483760550790 0.137408549828 T T T
 0.277780000000 0.555560000000 0.067840000000 F F F
 0.222220000000 0.611110000000 0.000000000000 F F F
 0.611110000000 0.555560000000 0.067840000000 F F F
 0.652356448736 0.489591972107 0.168379837119 T T T
 0.777780000000 0.555560000000 0.067840000000 F F F
 0.489618629681 0.644632620085 0.138029179653 T T T
 0.611110000000 0.388890000000 0.067840000000 F F F
 0.944440000000 0.555560000000 0.067840000000 F F F
 0.888890000000 0.611110000000 0.000000000000 F F F
 0.986144024502 0.643317978174 0.137260045781 T T T
 0.111110000000 0.722220000000 0.067840000000 F F F
 0.055560000000 0.777780000000 0.000000000000 F F F
 0.157807270714 0.646929156488 0.135770249245 T T T
 0.277780000000 0.722220000000 0.067840000000 F F F
 0.222220000000 0.777780000000 0.000000000000 F F F
 0.328012651056 0.647066856164 0.137504493170 T T T
 0.444440000000 0.722220000000 0.067840000000 F F F
 0.777780000000 0.055560000000 0.067840000000 F F F
 0.555560000000 0.444440000000 0.000000000000 F F F
 0.654277164124 0.317003098650 0.137150730088 T T T
 0.991684635957 0.481000210242 0.135575926980 T T T
 0.816052504454 0.480649847574 0.135603883522 T T T
 0.388890000000 0.611110000000 0.000000000000 F F F
 0.722220000000 0.611110000000 0.000000000000 F F F
 0.888890000000 0.944440000000 0.000000000000 F F F
 0.555560000000 0.777780000000 0.000000000000 F F F
 0.65295355127 0.641275126170 0.136148154139 T T T
 0.777780000000 0.722220000000 0.067840000000 F F F
 0.611110000000 0.722220000000 0.067840000000 F F F
 0.444440000000 0.555560000000 0.067840000000 F F F
 0.944440000000 0.722220000000 0.067840000000 F F F
 0.888890000000 0.777780000000 0.000000000000 F F F
 0.111110000000 0.888890000000 0.067840000000 F F F
 0.055560000000 0.944440000000 0.000000000000 F F F
 0.150341664198 0.816919884319 0.137901450806 T T T
 0.493570937599 0.483201061193 0.137138072195 T T T
 0.111110000000 0.555560000000 0.067840000000 F F F
 0.327173451831 0.481327346146 0.136728365057 T T T
 0.777780000000 0.888890000000 0.067840000000 F F F
 0.388890000000 0.944440000000 0.000000000000 F F F

0.444440000000 0.888890000000 0.067840000000 F F F
 0.817367172953 0.805313341264 0.135892740619 T T T
 0.722220000000 0.944440000000 0.000000000000 F F F
 0.722220000000 0.777780000000 0.000000000000 F F F
 0.222220000000 0.944440000000 0.000000000000 F F F
 0.491454945523 0.808665318572 0.138628288871 T T T
 0.555560000000 0.944440000000 0.000000000000 F F F
 0.611110000000 0.888890000000 0.067840000000 F F F
 0.660849800545 0.813579375954 0.136975864037 T T T
 0.179997016962 0.532924961586 0.194026763098 T T T
 0.670789962032 0.275523533479 0.477240599617 T T T
 0.748710652275 0.594332140229 0.196898917211 T T T
 0.541031215995 0.317432933293 0.502636535440 T T T
 0.709110915004 0.129670816273 0.210624501793 T T T
 0.969627574917 0.301470576385 0.193752816285 T T T
 0.002222093238 0.645639003764 0.194201257525 T T T
 0.810944909553 0.386259884520 0.186663600568 T T T
 0.155466425516 0.079449355893 0.184982323262 T T T
 0.509945096889 0.936686759973 0.185378382267 T T T
 0.227877372641 0.823450762389 0.183681622547 T T T
 0.396825184307 0.066709099589 0.185111019241 T T T
 0.874361243985 0.035875053853 0.199951918171 T T T
 0.374971925737 0.269098780446 0.181308755368 T T T
 0.178129119789 0.313400761754 0.193781476255 T T T
 0.611678585888 0.330189009766 0.526579321975 T T T
 0.482889588937 0.375998515491 0.556602424481 T T T
 0.601244717365 0.263806563365 0.452369255554 T T T
 0.535843405064 0.472679987479 0.473970774892 T T T
 0.447844852486 0.709529935088 0.450979787470 T T T
 0.684337126556 0.837533187381 0.194371073840 T T T
 0.375743592321 0.388770616003 0.477379501074 T T T
 0.799812717570 0.260360424797 0.486559519321 T T T
 0.478485269530 0.031241502821 0.525335542355 T T T
 0.676155030742 0.309854506977 0.514465425773 T T T
 0.538131335332 0.284583793822 0.465063837274 T T T
 0.458213105588 0.398175801701 0.488206698966 T T T
 0.440207915767 0.907388573904 0.489180328488 T T T
 0.448700900488 0.525696289777 0.440730491712 T T T
 0.399574612888 0.762534070083 0.456493669633 T T T
 0.394763455248 0.627149694280 0.425542563467 T T T
 0.531842610799 0.535639485711 0.450469293490 T T T

0.379643952940 0.241196200720 0.517937320920 TTT
 0.466097938505 0.333577134734 0.516051042409 TTT
 0.370242317318 0.451312376055 0.453996415700 TTT
 0.545239350174 0.440517938667 0.557801234533 TTT
 0.428013055765 0.387851589938 0.564008867931 TTT
 0.485259515931 0.331503366047 0.578575454415 TTT
 0.836183850227 0.236211856967 0.469156186457 TTT
 0.392199837755 0.195443222741 0.535152247615 TTT
 0.598868774751 0.238416704676 0.423386950857 TTT
 0.616529333257 0.355439224755 0.555770416412 TTT
 0.729523352961 0.320050235365 0.534087181821 TTT
 0.484826292655 0.275401297559 0.445480867068 TTT
 0.773161046586 0.218972974122 0.512604500855 TTT
 0.495506302464 0.654413611548 0.486721063317 TTT
 0.357801627834 0.885627903789 0.441997035518 TTT
 0.357826882765 0.211611350316 0.489215958838 TTT
 0.313862630552 0.330966619783 0.486942093979 TTT
 0.383429838281 0.978516712311 0.469831218294 TTT
 0.486590126550 0.825517461754 0.503059137699 TTT
 0.377892495100 0.645716350854 0.397815587760 TTT
 0.393370599565 0.787417472983 0.428094021912 TTT
 0.331541881822 0.718359494742 0.467852377431 TTT
 0.512705783212 0.753248635674 0.436781305357 TTT
 0.324888088142 0.246394467667 0.531320269516 TTT
 0.845022544376 0.330488459029 0.494768809620 TTT
 0.305157893477 0.440901053269 0.445399428958 TTT
 0.592195265458 0.592414471084 0.438917614049 TTT
 0.600971521384 0.481237850244 0.481305753262 TTT
 0.332970448047 0.578453084563 0.440198832991 TTT
 0.191357969466 0.557156036549 0.226211276852 TTT
 0.516860388582 0.907782803643 0.215194041090 TTT
 0.152944669459 0.065290117138 0.218418911295 TTT
 0.440873140400 0.108023634327 0.211674180889 TTT
 0.184241730233 0.301026964244 0.226605953419 TTT
 0.008001841782 0.633913048991 0.227127651811 TTT
 0.272934528786 0.818793398044 0.208254488963 TTT
 0.692991074414 0.838449245198 0.227935973193 TTT
 0.665798267262 0.162538384466 0.202359636532 TTT
 0.925439006602 0.014895976427 0.188880751366 TTT
 0.395894189672 0.287001734535 0.214057717899 TTT
 0.798722418143 0.416565876368 0.214937331905 TTT

```

0.474887261931 0.095776396247 0.533289402887 TTT
0.485542184336 0.960356950743 0.518380087601 TTT
0.943227198535 0.272396982818 0.224626551452 TTT
0.451494568526 0.836544574652 0.482407823766 TTT
0.807756563179 0.661155319785 0.209977801248 TTT
0.383594096917 0.920333767404 0.466608004377 TTT
0.462180676418 0.685978085072 0.488944667357 TTT
0.729020543411 0.252190628864 0.462469600580 TTT
0.449670769179 0.589045463372 0.416369244324 TTT

```

The initial structure of the NEB chain for the model with the curing agent (coverage: 50 %)

Au 6 × 6 supercell (3 layers)

1.0

```

17.302800000000 0.000000000000 0.000000000000
-8.651400000000 14.984664356600 0.000000000000
0.000000000000 0.000000000000 34.709200000000

```

Au C H N O

108 39 26 22 3

Selective dynamics

Direct

```

0.013377234225 0.022589468451 0.137126000000 TTT
0.995789000000 0.831100000000 0.135799000000 TTT
0.111110000000 0.055560000000 0.067840000000 FFF
0.555560000000 0.611110000000 0.000000000000 FFF
0.055560000000 0.111110000000 0.000000000000 FFF
0.184291312333 0.011783978967 0.139732000000 TTT
0.277780000000 0.055560000000 0.067840000000 FFF
0.222220000000 0.111110000000 0.000000000000 FFF
0.337984000000 0.003116000000 0.136903000000 TTT
0.444440000000 0.055560000000 0.067840000000 FFF
0.502726000000 0.006292000000 0.137414000000 TTT
0.611110000000 0.055560000000 0.067840000000 FFF
0.555560000000 0.111110000000 0.000000000000 FFF
0.777780000000 0.055560000000 0.067840000000 FFF
0.444440000000 0.222220000000 0.067840000000 FFF
0.722220000000 0.111110000000 0.000000000000 FFF
0.888890000000 0.444440000000 0.000000000000 FFF
0.055560000000 0.277780000000 0.000000000000 FFF
0.168783000000 0.165401000000 0.135989000000 TTT
0.277780000000 0.222220000000 0.067840000000 FFF

```

0.222220000000 0.277780000000 0.000000000000 F F F
 0.335057000000 0.166902000000 0.136482000000 T T T
 0.658835000000 0.994474000000 0.138265000000 T T T
 0.111110000000 0.222220000000 0.067840000000 F F F
 0.944440000000 0.055560000000 0.067840000000 F F F
 0.888890000000 0.111110000000 0.000000000000 F F F
 0.003365411425 0.165402000000 0.136349000000 T T T
 0.000776000000 0.331522000000 0.136385000000 T T T
 0.055560000000 0.444440000000 0.000000000000 F F F
 0.944440000000 0.388890000000 0.067840000000 F F F
 0.722220000000 0.277780000000 0.000000000000 F F F
 0.888890000000 0.277780000000 0.000000000000 F F F
 0.444440000000 0.888890000000 0.067840000000 F F F
 0.830259000000 0.168049000000 0.137907000000 T T T
 0.492935000000 0.824085000000 0.135965000000 T T T
 0.111110000000 0.388890000000 0.067840000000 F F F
 0.944440000000 0.222220000000 0.067840000000 F F F
 0.555560000000 0.444440000000 0.000000000000 F F F
 0.667116000000 0.171051000000 0.134720000000 T T T
 0.692196000000 0.452885000000 0.208905000000 T T T
 0.611110000000 0.222220000000 0.067840000000 F F F
 0.164820000000 0.333292000000 0.137010000000 T T T
 0.222220000000 0.444440000000 0.000000000000 F F F
 0.326230000000 0.331676000000 0.142759000000 T T T
 0.444440000000 0.388890000000 0.067840000000 F F F
 0.388890000000 0.444440000000 0.000000000000 F F F
 0.502080000000 0.336771000000 0.134320000000 T T T
 0.388890000000 0.277780000000 0.000000000000 F F F
 0.277780000000 0.388890000000 0.067840000000 F F F
 0.777780000000 0.388890000000 0.067840000000 F F F
 0.722220000000 0.444440000000 0.000000000000 F F F
 0.508953000000 0.178981000000 0.138475000000 T T T
 0.839589234225 0.017945468451 0.137217000000 T T T
 0.388890000000 0.944440000000 0.000000000000 F F F
 0.824678000000 0.333230000000 0.134939000000 T T T
 0.777780000000 0.722220000000 0.067840000000 F F F
 0.498460000000 0.496413000000 0.137423000000 T T T
 0.824143000000 0.492042000000 0.137419000000 T T T
 0.004334822849 0.492596000000 0.137191000000 T T T
 0.388890000000 0.777780000000 0.000000000000 F F F
 0.055560000000 0.611110000000 0.000000000000 F F F

0.163583000000 0.497609000000 0.136187000000 T T T
 0.277780000000 0.555560000000 0.067840000000 F F F
 0.388890000000 0.611110000000 0.000000000000 F F F
 0.611110000000 0.555560000000 0.067840000000 F F F
 0.664959000000 0.494020000000 0.136592000000 T T T
 0.777780000000 0.555560000000 0.067840000000 F F F
 0.500519000000 0.664718000000 0.136387000000 T T T
 0.722220000000 0.611110000000 0.000000000000 F F F
 0.944440000000 0.555560000000 0.067840000000 F F F
 0.888890000000 0.611110000000 0.000000000000 F F F
 0.611110000000 0.388890000000 0.067840000000 F F F
 0.111110000000 0.722220000000 0.067840000000 F F F
 0.055560000000 0.777780000000 0.000000000000 F F F
 0.167404000000 0.667103000000 0.137708000000 T T T
 0.277780000000 0.722220000000 0.067840000000 F F F
 0.222220000000 0.777780000000 0.000000000000 F F F
 0.329913000000 0.665865000000 0.136479000000 T T T
 0.444440000000 0.722220000000 0.067840000000 F F F
 0.444440000000 0.555560000000 0.067840000000 F F F
 0.335575000000 0.506546000000 0.138382000000 T T T
 0.222220000000 0.611110000000 0.000000000000 F F F
 0.555560000000 0.944440000000 0.000000000000 F F F
 0.888890000000 0.944440000000 0.000000000000 F F F
 0.555560000000 0.777780000000 0.000000000000 F F F
 0.662916000000 0.661417000000 0.136911000000 T T T
 0.944440000000 0.888890000000 0.067840000000 F F F
 0.611110000000 0.722220000000 0.067840000000 F F F
 0.827898000000 0.659901000000 0.137026000000 T T T
 0.944440000000 0.722220000000 0.067840000000 F F F
 0.888890000000 0.777780000000 0.000000000000 F F F
 0.111110000000 0.888890000000 0.067840000000 F F F
 0.055560000000 0.944440000000 0.000000000000 F F F
 0.277780000000 0.888890000000 0.067840000000 F F F
 0.995033000000 0.661690000000 0.138336000000 T T T
 0.777780000000 0.888890000000 0.067840000000 F F F
 0.164327000000 0.830342000000 0.135900000000 T T T
 0.722220000000 0.777780000000 0.000000000000 F F F
 0.111110000000 0.555560000000 0.067840000000 F F F
 0.831850000000 0.830121000000 0.137752000000 T T T
 0.722220000000 0.944440000000 0.000000000000 F F F
 0.777780000000 0.222220000000 0.067840000000 F F F

0.663391000000 0.828139000000 0.139012000000 TTT
 0.555560000000 0.277780000000 0.000000000000 FFF
 0.222220000000 0.944440000000 0.000000000000 FFF
 0.611110000000 0.888890000000 0.067840000000 FFF
 0.332481000000 0.833712000000 0.135413000000 TTT
 0.388890000000 0.111110000000 0.000000000000 FFF
 0.724503000000 0.386109000000 0.291914000000 TTT
 0.004416000000 0.607501000000 0.353404000000 TTT
 0.351613000000 0.156386000000 0.193816000000 TTT
 0.627317000000 0.656896000000 0.192551000000 TTT
 0.160837000000 0.912090000000 0.183939000000 TTT
 0.492583000000 0.813326000000 0.193845000000 TTT
 0.893765000000 0.220387000000 0.188764000000 TTT
 0.010877000000 0.092936000000 0.183612000000 TTT
 0.350936000000 0.553576000000 0.192934000000 TTT
 0.990646000000 0.483185000000 0.195125000000 TTT
 0.003753000000 0.673641000000 0.196178000000 TTT
 0.790002000000 0.547754000000 0.289978000000 TTT
 0.934229000000 0.862564000000 0.184065000000 TTT
 0.764390000000 0.583572000000 0.208745000000 TTT
 0.651480000000 0.059508000000 0.185815000000 TTT
 0.617289000000 0.322591000000 0.201022000000 TTT
 0.393062000000 0.957715000000 0.181250000000 TTT
 0.207757000000 0.682165000000 0.193553000000 TTT
 0.428518000000 0.390597000000 0.185131000000 TTT
 0.476962000000 0.533013000000 0.299785000000 TTT
 0.149256000000 0.670248000000 0.329768000000 TTT
 0.171645000000 0.334955000000 0.194731000000 TTT
 0.752505000000 0.911946000000 0.184364000000 TTT
 0.314967000000 0.748864000000 0.319217000000 TTT
 0.721607000000 0.625612000000 0.328008000000 TTT
 0.789458000000 0.470641000000 0.277233000000 TTT
 0.766093000000 0.648125000000 0.368554000000 TTT
 0.723983000000 0.543290000000 0.314353000000 TTT
 0.353875000000 0.688577000000 0.304826000000 TTT
 0.660464000000 0.457874000000 0.328916000000 TTT
 0.599933000000 0.656006000000 0.352823000000 TTT
 0.514526000000 0.643578000000 0.351366000000 TTT
 0.626452000000 0.609225000000 0.327849000000 TTT
 0.776821000000 0.707187000000 0.301371000000 TTT
 0.563660000000 0.550382000000 0.300817000000 TTT

0.660786000000 0.381540000000 0.318642000000 TTT
 0.780859000000 0.305396000000 0.256333000000 TTT
 0.451813000000 0.580187000000 0.325242000000 TTT
 0.335381000000 0.617142000000 0.335389000000 TTT
 0.646723000000 0.702038000000 0.374245000000 TTT
 0.843169000000 0.611667000000 0.279835000000 TTT
 0.749594000000 0.694320000000 0.271902000000 TTT
 0.462914000000 0.762632000000 0.272946000000 TTT
 0.724818000000 0.598415000000 0.390170000000 TTT
 0.428523000000 0.488079000000 0.278875000000 TTT
 0.756999000000 0.234303000000 0.252206000000 TTT
 0.780028000000 0.335884000000 0.228550000000 TTT
 0.849470000000 0.340355000000 0.267938000000 TTT
 0.612909000000 0.316613000000 0.330589000000 TTT
 0.845676000000 0.477119000000 0.260431000000 TTT
 0.847805000000 0.726689000000 0.300352000000 TTT
 0.493970000000 0.679514000000 0.370535000000 TTT
 0.610466000000 0.452280000000 0.349704000000 TTT
 0.065196000000 0.633262000000 0.283281000000 TTT
 0.175957000000 0.677051000000 0.270819000000 TTT
 0.366510000000 0.648232000000 0.363026000000 TTT
 0.583532000000 0.517392000000 0.279480000000 TTT
 0.774033000000 0.765547000000 0.312383000000 TTT
 0.241103000000 0.719202000000 0.370734000000 TTT
 0.368831000000 0.801241000000 0.336826000000 TTT
 0.307167000000 0.782477000000 0.293478000000 TTT
 0.322310000000 0.657129000000 0.277414000000 TTT
 0.780490000000 0.714039000000 0.378834000000 TTT
 0.262971000000 0.575658000000 0.339310000000 TTT
 0.828835000000 0.647694000000 0.366261000000 TTT
 0.388197000000 0.935342000000 0.213916000000 TTT
 0.607635000000 0.655469000000 0.224984000000 TTT
 0.361994000000 0.580780000000 0.224794000000 TTT
 0.179904000000 0.337902000000 0.228386000000 TTT
 0.652023000000 0.100452000000 0.213054000000 TTT
 0.021642000000 0.100478000000 0.217342000000 TTT
 0.938555000000 0.869392000000 0.218048000000 TTT
 0.933304000000 0.255642000000 0.217156000000 TTT
 0.461718000000 0.401825000000 0.216122000000 TTT
 0.747912000000 0.911205000000 0.218451000000 TTT
 0.367330000000 0.142166000000 0.225141000000 TTT

```

0.983016000000 0.474529000000 0.228626000000 TTT
0.810422000000 0.660063000000 0.201975000000 TTT
0.925508000000 0.574182000000 0.352223000000 TTT
0.488595000000 0.801678000000 0.227048000000 TTT
0.237902000000 0.694021000000 0.224704000000 TTT
0.574704000000 0.247580000000 0.191234000000 TTT
0.089911000000 0.642578000000 0.358845000000 TTT
0.235312000000 0.709226000000 0.341929000000 TTT
0.011031000000 0.687672000000 0.229488000000 TTT
0.169315000000 0.901381000000 0.217048000000 TTT
0.129470000000 0.658745000000 0.292488000000 TTT
0.445661000000 0.744735000000 0.300642000000 TTT
0.719027000000 0.308429000000 0.282639000000 TTT
0.365513000000 0.558395000000 0.322477000000 TTT

```

The final structure of the NEB chain for the model with the curing agent (coverage: 50 %)

Au 6 × 6 supercell (3 layers)

1.0

```

17.302800000000 0.000000000000 0.000000000000
-8.651400000000 14.984664356600 0.000000000000
0.000000000000 0.000000000000 34.709200000000

```

Au C H N O

108 39 26 22 3

Selective dynamics

Direct

```

0.000370505322 -0.002058211396 0.137915468145 TTT
0.997753817603 0.830396212925 0.136868008004 TTT
0.111110000000 0.055560000000 0.067840000000 FFF
0.555560000000 0.611110000000 0.000000000000 FFF
0.055560000000 0.111110000000 0.000000000000 FFF
0.167506101148 0.001122988098 0.135818514196 TTT
0.277780000000 0.055560000000 0.067840000000 FFF
0.222220000000 0.111110000000 0.000000000000 FFF
0.335081609316 0.000906091754 0.137920311208 TTT
0.444440000000 0.055560000000 0.067840000000 FFF
0.499991130553 0.000859692593 0.135988362786 TTT
0.611110000000 0.055560000000 0.067840000000 FFF
0.555560000000 0.111110000000 0.000000000000 FFF
0.777780000000 0.055560000000 0.067840000000 FFF
0.444440000000 0.222220000000 0.067840000000 FFF

```

0.722220000000 0.111110000000 0.000000000000 F F F
 0.888890000000 0.444440000000 0.000000000000 F F F
 0.055560000000 0.277780000000 0.000000000000 F F F
 0.170570342727 0.167418341494 0.137578237169 T T T
 0.277780000000 0.222220000000 0.067840000000 F F F
 0.222220000000 0.277780000000 0.000000000000 F F F
 0.333712039837 0.166583766519 0.136943715209 T T T
 0.664423709482 0.998400963110 0.136808322630 T T T
 0.111110000000 0.222220000000 0.067840000000 F F F
 0.944440000000 0.055560000000 0.067840000000 F F F
 0.888890000000 0.111110000000 0.000000000000 F F F
 0.004968751946 0.164997706498 0.136465765690 T T T
 0.002584311146 0.332617480838 0.136166521912 T T T
 0.055560000000 0.444440000000 0.000000000000 F F F
 0.944440000000 0.388890000000 0.067840000000 F F F
 0.722220000000 0.277780000000 0.000000000000 F F F
 0.888890000000 0.277780000000 0.000000000000 F F F
 0.444440000000 0.888890000000 0.067840000000 F F F
 0.833288927822 0.167360263033 0.137410554921 T T T
 0.497160857249 0.830058114058 0.136252950648 T T T
 0.111110000000 0.388890000000 0.067840000000 F F F
 0.944440000000 0.222220000000 0.067840000000 F F F
 0.555560000000 0.444440000000 0.000000000000 F F F
 0.667319885960 0.172235211730 0.134469455506 T T T
 0.703707731989 0.439754038598 0.209033054951 T T T
 0.611110000000 0.222220000000 0.067840000000 F F F
 0.167939036247 0.332230674753 0.136598068462 T T T
 0.222220000000 0.444440000000 0.000000000000 F F F
 0.331948205306 0.332780259465 0.140870835196 T T T
 0.444440000000 0.388890000000 0.067840000000 F F F
 0.388890000000 0.444440000000 0.000000000000 F F F
 0.502843595951 0.333910112763 0.134212219442 T T T
 0.388890000000 0.277780000000 0.000000000000 F F F
 0.277780000000 0.388890000000 0.067840000000 F F F
 0.777780000000 0.388890000000 0.067840000000 F F F
 0.722220000000 0.444440000000 0.000000000000 F F F
 0.506246381594 0.172841471307 0.135368925063 T T T
 0.835231571695 0.001383621868 0.135370650523 T T T
 0.388890000000 0.944440000000 0.000000000000 F F F
 0.824983695914 0.331457083429 0.135873555865 T T T
 0.777780000000 0.722220000000 0.067840000000 F F F

0.500276646606 0.498384110774 0.136004747037 TTT
 0.825346352281 0.492599492818 0.135120476435 TTT
 0.010705692361 0.494801306295 0.139200477113 TTT
 0.388890000000 0.777780000000 0.000000000000 FFFF
 0.055560000000 0.611110000000 0.000000000000 FFFF
 0.163178439145 0.496523471869 0.136166535025 TTT
 0.277780000000 0.555560000000 0.067840000000 FFFF
 0.388890000000 0.611110000000 0.000000000000 FFFF
 0.611110000000 0.555560000000 0.067840000000 FFFF
 0.664719937138 0.491696014384 0.135754233606 TTT
 0.777780000000 0.555560000000 0.067840000000 FFFF
 0.498068719045 0.665516177886 0.137837193214 TTT
 0.722220000000 0.611110000000 0.000000000000 FFFF
 0.944440000000 0.555560000000 0.067840000000 FFFF
 0.888890000000 0.611110000000 0.000000000000 FFFF
 0.611110000000 0.388890000000 0.067840000000 FFFF
 0.111110000000 0.722220000000 0.067840000000 FFFF
 0.055560000000 0.777780000000 0.000000000000 FFFF
 0.160770793902 0.660014041529 0.138464868994 TTT
 0.277780000000 0.722220000000 0.067840000000 FFFF
 0.222220000000 0.777780000000 0.000000000000 FFFF
 0.327007573216 0.662971623627 0.138249225342 TTT
 0.444440000000 0.722220000000 0.067840000000 FFFF
 0.444440000000 0.555560000000 0.067840000000 FFFF
 0.331689613685 0.500677574506 0.136781392112 TTT
 0.222220000000 0.611110000000 0.000000000000 FFFF
 0.555560000000 0.944440000000 0.000000000000 FFFF
 0.888890000000 0.944440000000 0.000000000000 FFFF
 0.555560000000 0.777780000000 0.000000000000 FFFF
 0.662448915530 0.660773061021 0.137163515948 TTT
 0.944440000000 0.888890000000 0.067840000000 FFFF
 0.611110000000 0.722220000000 0.067840000000 FFFF
 0.829108175912 0.660484845797 0.136730772571 TTT
 0.944440000000 0.722220000000 0.067840000000 FFFF
 0.888890000000 0.777780000000 0.000000000000 FFFF
 0.111110000000 0.888890000000 0.067840000000 FFFF
 0.055560000000 0.944440000000 0.000000000000 FFFF
 0.277780000000 0.888890000000 0.067840000000 FFFF
 0.997434483898 0.662587803757 0.136496609264 TTT
 0.777780000000 0.888890000000 0.067840000000 FFFF
 0.164879657972 0.831387302553 0.136729290717 TTT

0.722220000000 0.777780000000 0.000000000000 F F F
 0.111110000000 0.555560000000 0.067840000000 F F F
 0.831807311324 0.830049923841 0.136213415890 T T T
 0.722220000000 0.944440000000 0.000000000000 F F F
 0.777780000000 0.222220000000 0.067840000000 F F F
 0.664919654107 0.828167567632 0.138635666762 T T T
 0.555560000000 0.277780000000 0.000000000000 F F F
 0.222220000000 0.944440000000 0.000000000000 F F F
 0.611110000000 0.888890000000 0.067840000000 F F F
 0.329875331206 0.830330052316 0.136056901638 T T T
 0.388890000000 0.111110000000 0.000000000000 F F F
 0.720404706141 0.376758000879 0.509736309664 T T T
 0.010406949454 0.616776572147 0.570943780561 T T T
 0.335499082075 0.159225882489 0.194532909854 T T T
 0.639994444208 0.653340052744 0.194128000675 T T T
 0.165392500956 0.899976990379 0.185066983550 T T T
 0.511884313000 0.834137346161 0.193685272245 T T T
 0.909243386452 0.226702569753 0.185520494856 T T T
 0.051898947872 0.102118836085 0.180648663011 T T T
 0.387652720514 0.577068654648 0.185467437075 T T T
 0.912614887313 0.435969892103 0.185186757657 T T T
 0.020913992624 0.666966569992 0.193506148952 T T T
 0.768665122714 0.532054105122 0.497983116755 T T T
 0.930250320824 0.856974312782 0.182462541121 T T T
 0.782568619751 0.570264019709 0.210628294565 T T T
 0.666242769250 0.071220914665 0.183760760677 T T T
 0.620070262309 0.311585141950 0.199979261602 T T T
 0.410084065555 0.993886965984 0.184037917298 T T T
 0.269396693175 0.719193017748 0.181360721031 T T T
 0.438182224835 0.389057170626 0.182121111925 T T T
 0.480299712391 0.543838964171 0.513703050725 T T T
 0.155855884238 0.683964416031 0.552358405052 T T T
 0.186079403282 0.347127512506 0.193884709030 T T T
 0.739878762492 0.901806925334 0.184994836947 T T T
 0.320756666537 0.757849824500 0.539155805434 T T T
 0.721770492373 0.619846696408 0.543007320315 T T T
 0.769390950080 0.454686611739 0.487710502913 T T T
 0.769107706245 0.645825609374 0.582697493545 T T T
 0.720151094322 0.534700372528 0.529843055202 T T T
 0.341849257078 0.686912200802 0.523631054805 T T T
 0.670006073708 0.455018047973 0.551055878059 T T T

0.595613802210 0.636332418348 0.574040535183 TTT
 0.510325264702 0.625934764629 0.573619333747 TTT
 0.625832661281 0.602555527778 0.544588108398 TTT
 0.774937276957 0.699212480665 0.515343150478 TTT
 0.565576818618 0.555217960569 0.514588987449 TTT
 0.669812251819 0.377458107727 0.541478288948 TTT
 0.768563019774 0.292619847680 0.471642190097 TTT
 0.452408552006 0.580301293276 0.543033627494 TTT
 0.343678743334 0.627184427722 0.555862547771 TTT
 0.639388819352 0.672285538983 0.598082727954 TTT
 0.807739586607 0.591836265068 0.480772008724 TTT
 0.747719667476 0.684953424250 0.485955256309 TTT
 0.439452835475 0.698555543253 0.490323519559 TTT
 0.730128457830 0.596808117774 0.605106270304 TTT
 0.434271201382 0.507460048458 0.490307652164 TTT
 0.756673636918 0.224273446481 0.472286254024 TTT
 0.746274316380 0.305074595478 0.443827647244 TTT
 0.840148529569 0.339879183798 0.475706644325 TTT
 0.631657137615 0.316198263309 0.557975673655 TTT
 0.808283134083 0.455571337408 0.462900719772 TTT
 0.845554806671 0.717324694537 0.514206575130 TTT
 0.490007977610 0.653228248526 0.597281411301 TTT
 0.630412224926 0.454629301518 0.575597868018 TTT
 0.071307009019 0.649971943212 0.506671337694 TTT
 0.183125607697 0.706445811101 0.493768631390 TTT
 0.391027841624 0.668629679917 0.578365660106 TTT
 0.586446943095 0.527353360959 0.491298535604 TTT
 0.771929754787 0.757555464391 0.525786256461 TTT
 0.250114065292 0.727382899373 0.592534165770 TTT
 0.378785079962 0.806057524735 0.556028677161 TTT
 0.316618362326 0.795952138938 0.514592916928 TTT
 0.291221970218 0.643764949238 0.502202342367 TTT
 0.780775109408 0.711555152049 0.592013430235 TTT
 0.277140387381 0.587286229545 0.568770177435 TTT
 0.833743463301 0.648640574353 0.580494710728 TTT
 0.424569931778 0.987978299928 0.216856980152 TTT
 0.624841662039 0.645920386708 0.227295816488 TTT
 0.404594963011 0.603269994896 0.217518441820 TTT
 0.200845157103 0.360088016275 0.226972508440 TTT
 0.668586667673 0.118235498921 0.209051802655 TTT
 0.062176912044 0.119005593616 0.214047305099 TTT

```

0.927112204970 0.865310548899 0.216174193779 TTT
0.948368645310 0.259816265174 0.214281512352 TTT
0.470303136259 0.397109233521 0.213092104554 TTT
0.788382040107 0.953979078253 0.208087884904 TTT
0.339793440889 0.156491596524 0.228184709661 TTT
0.867407002380 0.409988866935 0.213099884075 TTT
0.826017473934 0.645558990624 0.201179507321 TTT
0.933239998435 0.582614605295 0.564432348704 TTT
0.524758891643 0.838505307953 0.227007325155 TTT
0.273197066443 0.727513676587 0.215371890131 TTT
0.568912672005 0.240013019334 0.188460162516 TTT
0.095365697556 0.654225654763 0.580191805854 TTT
0.242707336562 0.724784144792 0.563528171162 TTT
0.036411743039 0.667075598904 0.226425478429 TTT
0.163157959126 0.939243379559 0.212521643769 TTT
0.136063133259 0.674596082967 0.514232748998 TTT
0.426999035291 0.738039686497 0.505797560590 TTT
0.717171910065 0.298032617938 0.502929120742 TTT
0.366671895279 0.565069783477 0.539746828646 TTT

```

The initial structure of the NEB chain for the model with the curing agent (coverage: 67 %)

Au 6 × 6 supercell (3 layers)

1.0

```

17.302800000000 0.000000000000 0.000000000000
-8.651400000000 14.984664356600 0.000000000000
0.000000000000 0.000000000000 34.709200000000

```

Au C H N O

108 45 26 28 3

Selective dynamics

Direct

```

0.938299785118 0.877687868810 0.144112355878 TTT
0.444440000000 0.888890000000 0.067840000000 FFF
0.111110000000 0.055560000000 0.067840000000 FFF
0.555560000000 0.611110000000 0.000000000000 FFF
0.126119324743 0.979813886938 0.135820620829 TTT
0.277780000000 0.055560000000 0.067840000000 FFF
0.222220000000 0.111110000000 0.000000000000 FFF
0.307182206243 0.046147370805 0.144019267741 TTT
0.444440000000 0.055560000000 0.067840000000 FFF
0.388890000000 0.111110000000 0.000000000000 FFF

```

0.393881031666 0.942430142804 0.134035172977 TTT
 0.611110000000 0.055560000000 0.067840000000 FFF
 0.555560000000 0.111110000000 0.000000000000 FFF
 0.777780000000 0.055560000000 0.067840000000 FFF
 0.444440000000 0.222220000000 0.067840000000 FFF
 0.722220000000 0.111110000000 0.000000000000 FFF
 0.944440000000 0.055560000000 0.067840000000 FFF
 0.888890000000 0.111110000000 0.000000000000 FFF
 0.989988108440 0.162043419380 0.136048348040 TTT
 0.055560000000 0.277780000000 0.000000000000 FFF
 0.149559070853 0.152331276128 0.138033640046 TTT
 0.277780000000 0.222220000000 0.067840000000 FFF
 0.222220000000 0.277780000000 0.000000000000 FFF
 0.488741383485 0.304721322992 0.261089225352 TTT
 0.655875047305 0.155560793960 0.135052785368 TTT
 0.111110000000 0.222220000000 0.067840000000 FFF
 0.925471386822 0.761766972171 0.208273065671 TTT
 0.611110000000 0.222220000000 0.067840000000 FFF
 0.944440000000 0.222220000000 0.067840000000 FFF
 0.826440165295 0.324531798324 0.135383393286 TTT
 0.998174482080 0.334974990123 0.137766456143 TTT
 0.817666845029 0.151321679141 0.137323943820 TTT
 0.888890000000 0.277780000000 0.000000000000 FFF
 0.111110000000 0.388890000000 0.067840000000 FFF
 0.777780000000 0.222220000000 0.067840000000 FFF
 0.277780000000 0.388890000000 0.067840000000 FFF
 0.555560000000 0.277780000000 0.000000000000 FFF
 0.944440000000 0.388890000000 0.067840000000 FFF
 0.712525361884 0.220160821387 0.261991377187 TTT
 0.555560000000 0.444440000000 0.000000000000 FFF
 0.661127192026 0.328923354600 0.134433208417 TTT
 0.165588890567 0.321989720524 0.134930072063 TTT
 0.222220000000 0.444440000000 0.000000000000 FFF
 0.328858691909 0.291614878160 0.138931045457 TTT
 0.444440000000 0.388890000000 0.067840000000 FFF
 0.388890000000 0.444440000000 0.000000000000 FFF
 0.504273588109 0.339083882513 0.133469369437 TTT
 0.388890000000 0.277780000000 0.000000000000 FFF
 0.888890000000 0.444440000000 0.000000000000 FFF
 0.839024338634 0.990315507045 0.135603738046 TTT
 0.722220000000 0.444440000000 0.000000000000 FFF

0.491119031280 0.161673118041 0.136435232341 TTT
 0.777780000000 0.388890000000 0.067840000000 FFF
 0.611110000000 0.888890000000 0.067840000000 FFF
 0.722220000000 0.277780000000 0.000000000000 FFF
 0.111110000000 0.888890000000 0.067840000000 FFF
 0.388890000000 0.777780000000 0.000000000000 FFF
 0.055560000000 0.611110000000 0.000000000000 FFF
 0.170108164580 0.508757352051 0.137462520486 TTT
 0.277780000000 0.555560000000 0.067840000000 FFF
 0.222220000000 0.611110000000 0.000000000000 FFF
 0.342104687680 0.501787119155 0.134798240734 TTT
 0.444440000000 0.555560000000 0.067840000000 FFF
 0.388890000000 0.611110000000 0.000000000000 FFF
 0.777780000000 0.555560000000 0.067840000000 FFF
 0.549601116307 0.757634336480 0.134970840128 TTT
 0.722220000000 0.611110000000 0.000000000000 FFF
 0.944440000000 0.555560000000 0.067840000000 FFF
 0.888890000000 0.611110000000 0.000000000000 FFF
 0.000979225342 0.685018372952 0.135483111474 TTT
 0.111110000000 0.722220000000 0.067840000000 FFF
 0.055560000000 0.777780000000 0.000000000000 FFF
 0.184061761476 0.689075672004 0.135316210640 TTT
 0.277780000000 0.722220000000 0.067840000000 FFF
 0.222220000000 0.777780000000 0.000000000000 FFF
 0.611110000000 0.388890000000 0.067840000000 FFF
 0.444440000000 0.722220000000 0.067840000000 FFF
 0.055560000000 0.111110000000 0.000000000000 FFF
 0.055560000000 0.444440000000 0.000000000000 FFF
 0.000169647830 0.501337995146 0.135137831275 TTT
 0.830434616985 0.510371755662 0.136386539531 TTT
 0.670052353235 0.512482008369 0.135376592342 TTT
 0.347602507123 0.671433382239 0.133603782675 TTT
 0.888890000000 0.944440000000 0.000000000000 FFF
 0.672674859690 0.526676825138 0.215480646971 TTT
 0.777780000000 0.722220000000 0.067840000000 FFF
 0.611110000000 0.555560000000 0.067840000000 FFF
 0.837436769987 0.683298662069 0.136034702012 TTT
 0.944440000000 0.722220000000 0.067840000000 FFF
 0.888890000000 0.777780000000 0.000000000000 FFF
 0.055560000000 0.944440000000 0.000000000000 FFF
 0.181167972126 0.853637364570 0.136954930777 TTT

0.277780000000 0.888890000000 0.067840000000 F F F
 0.395334670239 0.815092997230 0.181460362422 T T T
 0.611110000000 0.722220000000 0.067840000000 F F F
 0.511675957426 0.518056100701 0.135576471022 T T T
 0.388890000000 0.944440000000 0.000000000000 F F F
 0.722220000000 0.777780000000 0.000000000000 F F F
 0.222220000000 0.944440000000 0.000000000000 F F F
 0.555560000000 0.944440000000 0.000000000000 F F F
 0.741593517818 0.789908324402 0.134680659973 T T T
 0.687158469505 0.892113670046 0.179965185915 T T T
 0.722220000000 0.944440000000 0.000000000000 F F F
 0.777780000000 0.888890000000 0.067840000000 F F F
 0.555560000000 0.777780000000 0.000000000000 F F F
 0.944440000000 0.888890000000 0.067840000000 F F F
 0.111110000000 0.555560000000 0.067840000000 F F F
 0.577955832185 0.956703866503 0.135318534203 T T T
 0.172576389842 0.075594499339 0.180691057757 T T T
 0.402883096489 0.133500626643 0.183594720168 T T T
 0.408084312411 0.312792885252 0.224485760051 T T T
 0.145184338670 0.856285835094 0.191940378238 T T T
 0.201797327499 0.710456791550 0.192316942438 T T T
 0.958367821184 0.894835165706 0.203578970855 T T T
 0.165286588895 0.513779539091 0.195422066873 T T T
 0.039812769386 0.163430054483 0.188549338431 T T T
 0.377827420171 0.694228015469 0.195731133608 T T T
 0.699620188599 0.649468132560 0.203557484712 T T T
 0.489596298638 0.522771637370 0.191656715007 T T T
 0.635233240034 0.262442852113 0.285016464352 T T T
 0.992856300106 0.326689817210 0.195491836902 T T T
 0.009706421720 0.616521099241 0.180982825604 T T T
 0.642544095216 0.401826162077 0.210262820119 T T T
 0.876408388697 0.644823380664 0.233827904052 T T T
 0.813354092136 0.986146977702 0.197057709186 T T T
 0.573119857112 0.760925390155 0.193645296576 T T T
 0.583277399670 0.136583916055 0.183317370010 T T T
 0.830681820809 0.435016837610 0.181755104049 T T T
 0.381914158547 0.925246488122 0.194698249097 T T T
 0.771307666345 0.178760423131 0.224794306468 T T T
 0.271742631226 0.423890941505 0.179836467453 T T T
 0.297881439928 0.072031850331 0.303396604224 T T T
 0.589763391850 0.954341709007 0.193457383446 T T T

0.282803934251 0.189648086684 0.332699730180 TTT
 0.232485252099 0.899553990650 0.352268247758 TTT
 0.143624394177 0.203335153159 0.324577158544 TTT
 0.436106096294 0.070553526700 0.301021096053 TTT
 0.276944074434 0.335155252151 0.290370264638 TTT
 0.194574536911 0.154050609105 0.317405317830 TTT
 0.198341794640 0.301159907368 0.313011641060 TTT
 0.207173556336 0.031546839135 0.290589557053 TTT
 0.346360768125 0.642177366650 0.302051547769 TTT
 0.126452014594 0.197094380149 0.369270888485 TTT
 0.051218006308 0.160000882502 0.304674302852 TTT
 0.309477416663 0.841440190012 0.321071893264 TTT
 0.307188552299 0.486040412470 0.300406577110 TTT
 0.171494583444 0.362541081380 0.325340198778 TTT
 0.222882685164 0.452816945478 0.318627634649 TTT
 0.332454336838 0.425642267501 0.285226749780 TTT
 0.424584655561 0.810521348597 0.292120123931 TTT
 0.334511236680 0.151279654635 0.325641608704 TTT
 0.157700359317 0.073169702901 0.297340596790 TTT
 0.435243147871 0.729289195402 0.300515715605 TTT
 0.538619705227 0.745610730279 0.330955135784 TTT
 0.091467686677 0.043751560841 0.284676356716 TTT
 0.385731666907 0.798890843489 0.265698352332 TTT
 0.491488622678 0.868158925859 0.286859428015 TTT
 0.180836494423 0.971650098867 0.272893794848 TTT
 0.417575182500 0.856013419094 0.348158876122 TTT
 0.474097292237 0.724027718598 0.276583186378 TTT
 0.310835937528 0.250107088727 0.350161808213 TTT
 0.108316639718 0.338213048709 0.340436005084 TTT
 0.260792629488 0.776613715686 0.268291596928 TTT
 0.206540987375 0.828256948916 0.288290011645 TTT
 0.301159251110 0.636460787242 0.278422198926 TTT
 0.057376902596 0.157730307318 0.273384097779 TTT
 0.092317568625 0.126674887146 0.377921115082 TTT
 0.008201364142 0.091999238635 0.315624589426 TTT
 0.445847461540 0.068789524949 0.332190637673 TTT
 0.083212549682 0.224518911942 0.376512078265 TTT
 0.188572975038 0.233291356591 0.385835868366 TTT
 0.199544857781 0.497864788198 0.327602451671 TTT
 0.457063315213 0.029595589308 0.285157839623 TTT
 0.018238662025 0.198836323796 0.310682025786 TTT

0.402116625676 0.181356373094 0.336920416502 TTT
 0.313819158989 0.634860376153 0.330119367623 TTT
 0.293625896213 0.288967263583 0.276411035904 TTT
 0.472154553267 0.138828959678 0.289800944842 TTT
 0.393989077866 0.452905953700 0.268458697557 TTT
 0.071666344270 0.169507747588 0.219042680307 TTT
 0.395584930793 0.144517180517 0.216606064897 TTT
 0.838255256309 0.577558620316 0.251075165882 TTT
 0.201362618166 0.091041988597 0.212351608541 TTT
 0.368018918226 0.309379977185 0.196588517669 TTT
 0.717717869700 0.714937178580 0.186548770656 TTT
 0.366156113383 0.948267497274 0.224234690496 TTT
 0.580976964629 0.284105971066 0.287957987895 TTT
 0.633346708478 0.336669620993 0.195181031813 TTT
 0.165992766590 0.518710139710 0.229035208940 TTT
 0.221676403611 0.366265151570 0.200747782442 TTT
 0.988776071423 0.316931504829 0.228975779065 TTT
 0.560838645226 0.121699117921 0.215749918147 TTT
 0.978025612977 0.949003698948 0.228031483958 TTT
 0.174916062019 0.917957866222 0.354811312995 TTT
 0.475614587290 0.522541379947 0.224745750023 TTT
 0.569011283166 0.743345071195 0.226718996088 TTT
 0.829187540172 0.376762678590 0.200408245233 TTT
 0.299497407677 0.885850466679 0.351323585445 TTT
 0.252830697771 0.809109999430 0.291737013820 TTT
 0.011180059219 0.562822887288 0.201680572478 TTT
 0.382806693120 0.832951606811 0.323203228210 TTT
 0.118001544567 0.854698668381 0.223086040837 TTT
 0.850981562410 0.019531677662 0.226055109980 TTT
 0.367714625166 0.633502210503 0.214888801013 TTT
 0.793615309599 0.158071886745 0.196505123221 TTT
 0.211517638388 0.723567128706 0.225474615199 TTT
 0.590455014104 0.954035856749 0.227450917250 TTT
 0.482033320360 0.742472051807 0.336386409727 TTT
 0.341932534823 0.031238221564 0.292482607094 TTT
 0.367590881798 0.572007174957 0.296529571231 TTT

The final structure of the NEB chain for the model with the curing agent (coverage: 67 %)

Au 6 × 6 supercell (3 layers)

1.0

17.302800000000 0.000000000000 0.000000000000
 -8.651400000000 14.984664356600 0.000000000000
 0.000000000000 0.000000000000 34.709200000000
 Au C H N O
 108 45 26 28 3
 Selective dynamics
 Direct
 0.938007117682 0.880322643480 0.144069365138 TTT
 0.444440000000 0.888890000000 0.067840000000 FFF
 0.111110000000 0.055560000000 0.067840000000 FFF
 0.555560000000 0.611110000000 0.000000000000 FFF
 0.127109661513 0.978662501076 0.135418692218 TTT
 0.277780000000 0.055560000000 0.067840000000 FFF
 0.222220000000 0.111110000000 0.000000000000 FFF
 0.307970804108 0.046565408735 0.144219166073 TTT
 0.444440000000 0.055560000000 0.067840000000 FFF
 0.388890000000 0.111110000000 0.000000000000 FFF
 0.389916089311 0.935713996159 0.134884308699 TTT
 0.611110000000 0.055560000000 0.067840000000 FFF
 0.555560000000 0.111110000000 0.000000000000 FFF
 0.777780000000 0.055560000000 0.067840000000 FFF
 0.444440000000 0.222220000000 0.067840000000 FFF
 0.722220000000 0.111110000000 0.000000000000 FFF
 0.944440000000 0.055560000000 0.067840000000 FFF
 0.888890000000 0.111110000000 0.000000000000 FFF
 0.988796045505 0.163724009739 0.136031105217 TTT
 0.055560000000 0.277780000000 0.000000000000 FFF
 0.141075782426 0.146295586836 0.142449927794 TTT
 0.277780000000 0.222220000000 0.067840000000 FFF
 0.222220000000 0.277780000000 0.000000000000 FFF
 0.482034956146 0.301390654549 0.260975203401 TTT
 0.659366440521 0.157690768429 0.134650118037 TTT
 0.111110000000 0.222220000000 0.067840000000 FFF
 0.930573898510 0.762570374574 0.208358473875 TTT
 0.611110000000 0.222220000000 0.067840000000 FFF
 0.944440000000 0.222220000000 0.067840000000 FFF
 0.828854786782 0.326868156931 0.135242261083 TTT
 0.989433597684 0.336186823638 0.136843525539 TTT
 0.817865152176 0.151704002686 0.136899743037 TTT
 0.888890000000 0.277780000000 0.000000000000 FFF
 0.111110000000 0.388890000000 0.067840000000 FFF

0.777780000000 0.222220000000 0.067840000000 F F F
 0.277780000000 0.388890000000 0.067840000000 F F F
 0.555560000000 0.277780000000 0.000000000000 F F F
 0.944440000000 0.388890000000 0.067840000000 F F F
 0.704943130528 0.216889386051 0.259740837799 T T T
 0.555560000000 0.444440000000 0.000000000000 F F F
 0.660926642150 0.329279831998 0.134070836807 T T T
 0.167984655364 0.320463683720 0.135166581604 T T T
 0.222220000000 0.444440000000 0.000000000000 F F F
 0.323692769242 0.283186411332 0.139284486454 T T T
 0.444440000000 0.388890000000 0.067840000000 F F F
 0.388890000000 0.444440000000 0.000000000000 F F F
 0.501689161668 0.337703541948 0.133384846822 T T T
 0.388890000000 0.277780000000 0.000000000000 F F F
 0.888890000000 0.444440000000 0.000000000000 F F F
 0.837086205992 0.991253594958 0.135391882139 T T T
 0.722220000000 0.444440000000 0.000000000000 F F F
 0.492551590249 0.158111743060 0.136671713460 T T T
 0.777780000000 0.388890000000 0.067840000000 F F F
 0.611110000000 0.888890000000 0.067840000000 F F F
 0.722220000000 0.277780000000 0.000000000000 F F F
 0.111110000000 0.888890000000 0.067840000000 F F F
 0.388890000000 0.777780000000 0.000000000000 F F F
 0.055560000000 0.611110000000 0.000000000000 F F F
 0.171962268512 0.510424601657 0.136798506333 T T T
 0.277780000000 0.555560000000 0.067840000000 F F F
 0.222220000000 0.611110000000 0.000000000000 F F F
 0.340574383768 0.504646888155 0.135622030105 T T T
 0.444440000000 0.555560000000 0.067840000000 F F F
 0.388890000000 0.611110000000 0.000000000000 F F F
 0.777780000000 0.555560000000 0.067840000000 F F F
 0.548742445381 0.759795947524 0.134764103439 T T T
 0.722220000000 0.611110000000 0.000000000000 F F F
 0.944440000000 0.555560000000 0.067840000000 F F F
 0.888890000000 0.611110000000 0.000000000000 F F F
 0.000117325842 0.684089082084 0.135241416810 T T T
 0.111110000000 0.722220000000 0.067840000000 F F F
 0.055560000000 0.777780000000 0.000000000000 F F F
 0.182358229696 0.687471783153 0.136018337599 T T T
 0.277780000000 0.722220000000 0.067840000000 F F F
 0.222220000000 0.777780000000 0.000000000000 F F F

0.611110000000 0.388890000000 0.067840000000 F F F
 0.444440000000 0.722220000000 0.067840000000 F F F
 0.055560000000 0.111110000000 0.000000000000 F F F
 0.055560000000 0.444440000000 0.000000000000 F F F
 0.000673717475 0.501380481763 0.135372720755 T T T
 0.828651573202 0.510859178532 0.136801168859 T T T
 0.668130840237 0.512282185399 0.135444939701 T T T
 0.351040998327 0.677323991436 0.134799412184 T T T
 0.888890000000 0.944440000000 0.000000000000 F F F
 0.670527853845 0.524542730114 0.215184060519 T T T
 0.777780000000 0.722220000000 0.067840000000 F F F
 0.611110000000 0.555560000000 0.067840000000 F F F
 0.838605484002 0.686314042132 0.137004596750 T T T
 0.944440000000 0.722220000000 0.067840000000 F F F
 0.888890000000 0.777780000000 0.000000000000 F F F
 0.055560000000 0.944440000000 0.000000000000 F F F
 0.185596889021 0.854169147706 0.136727312039 T T T
 0.277780000000 0.888890000000 0.067840000000 F F F
 0.383942544669 0.809115235236 0.188136861410 T T T
 0.611110000000 0.722220000000 0.067840000000 F F F
 0.508090965374 0.516094088628 0.135161767394 T T T
 0.388890000000 0.944440000000 0.000000000000 F F F
 0.722220000000 0.777780000000 0.000000000000 F F F
 0.222220000000 0.944440000000 0.000000000000 F F F
 0.555560000000 0.944440000000 0.000000000000 F F F
 0.741148035395 0.790838557331 0.134632116945 T T T
 0.687412699739 0.890489110499 0.180985977261 T T T
 0.722220000000 0.944440000000 0.000000000000 F F F
 0.777780000000 0.888890000000 0.067840000000 F F F
 0.555560000000 0.777780000000 0.000000000000 F F F
 0.944440000000 0.888890000000 0.067840000000 F F F
 0.111110000000 0.555560000000 0.067840000000 F F F
 0.571705351412 0.955407710670 0.134596704902 T T T
 0.170123085669 0.069458726057 0.182289355697 T T T
 0.402231889419 0.134561076193 0.183348330283 T T T
 0.403879193499 0.312275053401 0.224102092350 T T T
 0.135892433111 0.851120493850 0.189380057671 T T T
 0.201461979441 0.715368213657 0.192724925643 T T T
 0.954001174011 0.895020851900 0.203060185638 T T T
 0.161067593661 0.515046685351 0.194048419352 T T T
 0.041469703561 0.158400654083 0.187680437799 T T T

0.373552905841 0.689128829780 0.198005228081 TTT
 0.698079014913 0.647207092411 0.202383833792 TTT
 0.490142763990 0.522295906320 0.191388136824 TTT
 0.628085386430 0.258829275263 0.284059328449 TTT
 0.989905286155 0.325043792839 0.194098380754 TTT
 0.007586812138 0.614627338042 0.180635394499 TTT
 0.636466102074 0.398554815690 0.209662606529 TTT
 0.871885450483 0.643089703121 0.232056035734 TTT
 0.812399735917 0.988451000845 0.196746320151 TTT
 0.572737092360 0.761452785138 0.193238141748 TTT
 0.577644028753 0.140034214759 0.180892312169 TTT
 0.826255145849 0.433099956268 0.181720476801 TTT
 0.382707433071 0.926134141183 0.196566851156 TTT
 0.768471735201 0.178934790994 0.223478583349 TTT
 0.270630281128 0.424286739315 0.180315061850 TTT
 0.307234844843 0.073638249524 0.501945865117 TTT
 0.592549252133 0.958021112344 0.191764362329 TTT
 0.276706298828 0.178271804688 0.534647890830 TTT
 0.239816975125 0.873469709889 0.557497023637 TTT
 0.144314904163 0.197893595904 0.518858228464 TTT
 0.438432651207 0.063472778711 0.513926280824 TTT
 0.270361972290 0.327466076065 0.482402073809 TTT
 0.198661277115 0.151068366529 0.512761432193 TTT
 0.205632982446 0.298316451825 0.511873826006 TTT
 0.228854867382 0.044241296736 0.480165106418 TTT
 0.345084668716 0.633912460691 0.489257631721 TTT
 0.106297900951 0.177156294638 0.560345738208 TTT
 0.064980388240 0.165288878761 0.490578442288 TTT
 0.309348327045 0.832965775458 0.512930971965 TTT
 0.314493486646 0.481380114863 0.494552837319 TTT
 0.196813391986 0.363717981092 0.532082426913 TTT
 0.249469906466 0.454435935086 0.523491212286 TTT
 0.324650904969 0.417229367431 0.474019961753 TTT
 0.400459655333 0.794714870336 0.468440248795 TTT
 0.330697419496 0.140868148860 0.529706503248 TTT
 0.175865879953 0.082633443042 0.485609629368 TTT
 0.422665035069 0.720330040621 0.473604594800 TTT
 0.513412248735 0.707618471040 0.502205075842 TTT
 0.116498832264 0.059578461081 0.467809912348 TTT
 0.343646402076 0.770881022275 0.448594492780 TTT
 0.458293567563 0.851841164503 0.454718562741 TTT

0.211959598219 0.992697407381 0.458428020498 TTT
 0.420629204366 0.831379812074 0.527403241419 TTT
 0.440289777824 0.705978794016 0.444899429007 TTT
 0.296546497371 0.231543296908 0.555811352529 TTT
 0.147522913210 0.344510970461 0.555025558484 TTT
 0.268447075738 0.829332561377 0.456741172829 TTT
 0.204695829185 0.840038833319 0.491739275104 TTT
 0.283285479962 0.613178159669 0.472731977721 TTT
 0.087030744615 0.176757960554 0.460404795428 TTT
 0.068352637510 0.104592978415 0.564616934184 TTT
 0.017174225715 0.093860527622 0.494597344565 TTT
 0.427210899388 0.050875596715 0.545048096304 TTT
 0.060616911848 0.202977327015 0.565501604999 TTT
 0.159096767918 0.205494880468 0.582274850148 TTT
 0.240372287968 0.503180088603 0.539756316554 TTT
 0.466450941505 0.024071623163 0.502146411590 TTT
 0.029736260666 0.202293518934 0.495865790686 TTT
 0.390287148906 0.164107260460 0.547330994279 TTT
 0.333204910741 0.641881854121 0.519811441652 TTT
 0.277744006953 0.278545571952 0.465379652482 TTT
 0.484777327204 0.134759273673 0.508525611326 TTT
 0.374120498256 0.439473642951 0.451041321387 TTT
 0.060698565693 0.162301236581 0.220458330420 TTT
 0.400161512317 0.150206169509 0.216301125487 TTT
 0.827774086071 0.575053005402 0.248175498842 TTT
 0.194890702461 0.076048167818 0.214497689197 TTT
 0.364623120573 0.307838704054 0.195796005277 TTT
 0.716198718906 0.712231476900 0.185042954970 TTT
 0.372584528468 0.961901780172 0.223505887187 TTT
 0.573809898371 0.280117818535 0.287529263868 TTT
 0.627114663244 0.333871716114 0.194039703503 TTT
 0.157339219201 0.518363395451 0.227648478293 TTT
 0.220427767883 0.366292816551 0.201089151644 TTT
 0.980426665963 0.314335801232 0.227466995412 TTT
 0.571024622668 0.127840639441 0.214510764015 TTT
 0.967498375105 0.943117189641 0.229573153866 TTT
 0.186294302223 0.893380031049 0.566602479204 TTT
 0.481779442008 0.523600940249 0.224897032123 TTT
 0.568240195729 0.739850501561 0.225815989497 TTT
 0.823773614827 0.374549290167 0.200487997540 TTT
 0.302186902918 0.853760655265 0.549128992318 TTT

```

0.249429799951 0.820515876003 0.484741151943 T T T
0.006805388067 0.559972692885 0.201483485462 T T T
0.379349699940 0.821349368656 0.504795841881 T T T
0.093650007469 0.840053028093 0.217463768234 T T T
0.850382375861 0.025385711148 0.225186815849 T T T
0.365451481863 0.626142459052 0.214809339799 T T T
0.792251840492 0.159247480077 0.195381802757 T T T
0.211160898299 0.732272845505 0.225788218304 T T T
0.602986942887 0.960426399084 0.225447758225 T T T
0.497997166256 0.754202635075 0.498931278224 T T T
0.355764753291 0.033534658118 0.493862567607 T T T
0.372526156053 0.568516543398 0.484598446699 T T T

```

Optimized 6×6 Au (111) surface structure on which a single cyanide is adsorbed

```

1.000000000000000
8.6514000000000006 -14.9846643566009998 0.000000000000000
8.6514000000000006 14.9846643566009998 0.000000000000000
0.000000000000000 0.000000000000000 34.709200000000027

```

Au C N

108 1 1

Selective dynamics

Direct

```

0.0000084664984744 -0.0000210070070232 0.1373059161106125 T T T
0.1111099999999965 0.0555599999999998 0.0678399999999968 F F F
0.5555599999999998 0.6111099999999965 0.000000000000000 F F F
0.0555599999999998 0.1111099999999965 0.000000000000000 F F F
0.1666058264353759 -0.0002025965709419 0.1375189411224967 T T T
0.2777799999999999 0.0555599999999998 0.0678399999999968 F F F
0.2222200000000001 0.1111099999999965 0.000000000000000 F F F
0.3331670214762322 -0.0002374649176049 0.1375026705349503 T T T
0.4444400000000002 0.0555599999999998 0.0678399999999968 F F F
0.3888900000000035 0.1111099999999965 0.000000000000000 F F F
0.4999793501416370 -0.0000170354577184 0.1373079183632906 T T T
0.6111099999999965 0.0555599999999998 0.0678399999999968 F F F
0.5555599999999998 0.1111099999999965 0.000000000000000 F F F
0.7777799999999999 0.0555599999999998 0.0678399999999968 F F F
0.4444400000000002 0.2222200000000001 0.0678399999999968 F F F
0.7222200000000001 0.1111099999999965 0.000000000000000 F F F
0.8888900000000035 0.4444400000000002 0.000000000000000 F F F

```

0.9444400000000002 0.0555599999999998 0.067839999999968 F F F
 0.8888900000000035 0.111109999999965 0.0000000000000000 F F F
 -0.0003831399588923 0.1664910186942452 0.1374840310406750 T T T
 0.0555599999999998 0.2777799999999999 0.0000000000000000 F F F
 0.1655790512106205 0.1655722944063493 0.1378513762443443 T T T
 0.2777799999999999 0.2222000000000001 0.067839999999968 F F F
 0.2222000000000001 0.2777799999999999 0.0000000000000000 F F F
 0.6668821264220406 0.0003925481086858 0.1374842391330238 T T T
 0.1111099999999965 0.2222000000000001 0.067839999999968 F F F
 0.8335173185564431 0.0003762061610231 0.1374803720677093 T T T
 0.6111099999999965 0.2222000000000001 0.067839999999968 F F F
 0.7222000000000001 0.2777799999999999 0.0000000000000000 F F F
 0.7777799999999999 0.2222000000000001 0.067839999999968 F F F
 0.8333457844683103 0.1666536536450376 0.1376366963643599 T T T
 0.9444400000000002 0.2222000000000001 0.067839999999968 F F F
 0.1111099999999965 0.3888900000000035 0.067839999999968 F F F
 -0.0003440564782894 0.3331420140794503 0.1374808144418582 T T T
 0.2777799999999999 0.3888900000000035 0.067839999999968 F F F
 0.0555599999999998 0.4444400000000002 0.0000000000000000 F F F
 0.8888900000000035 0.2777799999999999 0.0000000000000000 F F F
 0.5555599999999998 0.2777799999999999 0.0000000000000000 F F F
 0.6668908398721864 0.1664766917961230 0.1374874998758279 T T T
 0.3330988540541802 0.1661946042714580 0.1374764125828792 T T T
 0.5555599999999998 0.4444400000000002 0.0000000000000000 F F F
 0.1651922586103757 0.3325861099484705 0.1377774509582817 T T T
 0.2222000000000001 0.4444400000000002 0.0000000000000000 F F F
 0.3305245624174734 0.3310753591271921 0.1366474160804923 T T T
 0.4444400000000002 0.3888900000000035 0.067839999999968 F F F
 0.3888900000000035 0.4444400000000002 0.0000000000000000 F F F
 0.5005849183538545 0.3310802226898294 0.1366295933708657 T T T
 0.3888900000000035 0.2777799999999999 0.0000000000000000 F F F
 0.6674410980797990 0.3325740825196047 0.1377747738697137 T T T
 0.7777799999999999 0.3888900000000035 0.067839999999968 F F F
 0.7222000000000001 0.4444400000000002 0.0000000000000000 F F F
 0.4999966317577576 0.1655660508552607 0.1378357895612135 T T T
 0.9444400000000002 0.3888900000000035 0.067839999999968 F F F
 0.8335872564554250 0.3330686212416125 0.1375389402186198 T T T
 0.0002221845612261 0.8333666360061313 0.1375636203843331 T T T

0.6111099999999965 0.3888900000000035 0.0678399999999968 F F F
 0.0555599999999998 0.6111099999999965 0.0000000000000000 F F F
 0.1656010497490828 0.5000114934633340 0.137803885519579 T T T
 0.2777799999999999 0.5555599999999998 0.0678399999999968 F F F
 0.2222200000000001 0.6111099999999965 0.0000000000000000 F F F
 0.3305362985518420 0.4994450832517608 0.1366429609130357 T T T
 0.4444400000000002 0.5555599999999998 0.0678399999999968 F F F
 0.3888900000000035 0.6111099999999965 0.0000000000000000 F F F
 0.6111099999999965 0.5555599999999998 0.0678399999999968 F F F
 0.6689866255866499 0.4994346101901899 0.1366194405070364 T T T
 0.7777799999999999 0.5555599999999998 0.0678399999999968 F F F
 0.7222200000000001 0.6111099999999965 0.0000000000000000 F F F
 0.8344531123389470 0.4999717900815928 0.1378130986319476 T T T
 0.9444400000000002 0.5555599999999998 0.0678399999999968 F F F
 0.8888900000000035 0.6111099999999965 0.0000000000000000 F F F
 0.0002583623631655 0.6668359236087544 0.1375035531129368 T T T
 0.1111099999999965 0.7222200000000001 0.0678399999999968 F F F
 0.0555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.1666423976630730 0.6668243332904970 0.1375273700542959 T T T
 0.2777799999999999 0.7222200000000001 0.0678399999999968 F F F
 0.2222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.3331249014552199 0.6668757383963252 0.1374713464585865 T T T
 0.4444400000000002 0.7222200000000001 0.0678399999999968 F F F
 0.0000135366152809 0.5000229906061220 0.1373087274469139 T T T
 0.3888900000000035 0.7777799999999999 0.0000000000000000 F F F
 0.5006106159613405 0.6695619920362873 0.1366346977131998 T T T
 0.4999899621947020 0.4999479884479162 0.1387875065675135 T T T
 0.7222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.7777799999999999 0.7222200000000001 0.0678399999999968 F F F
 0.6111099999999965 0.7222200000000001 0.0678399999999968 F F F
 0.8339243357458058 0.6668967385083850 0.1374967402389312 T T T
 0.9444400000000002 0.7222200000000001 0.0678399999999968 F F F
 0.8888900000000035 0.7777799999999999 0.0000000000000000 F F F
 0.1111099999999965 0.8888900000000035 0.0678399999999968 F F F
 0.0555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.1666706983345691 0.8333365412148117 0.1373141040792780 T T T
 0.2777799999999999 0.8888900000000035 0.0678399999999968 F F F
 0.3331860685270329 0.8333680147336442 0.1375265026063681 T T T

0.5555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.2222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.3888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.4444400000000002 0.8888900000000035 0.067839999999968 F F F
 0.8344630107992456 0.8344124424467679 0.1378146492212237 T T T
 0.7222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.7777799999999999 0.8888900000000035 0.067839999999968 F F F
 0.6674503012650242 0.8348942334985309 0.1377839661547621 T T T
 0.9444400000000002 0.8888900000000035 0.067839999999968 F F F
 0.5555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.6111099999999965 0.8888900000000035 0.067839999999968 F F F
 0.5000134626035008 0.8344257953083629 0.1378074631044569 T T T
 0.8888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.6689935438666538 0.6695531654571064 0.1366247580111704 T T T
 0.1111099999999965 0.5555599999999998 0.067839999999968 F F F
 0.5015549595890844 0.5023485401315037 0.1972058155637342 T T T
 0.5035357561544519 0.5054168683326902 0.2309884351859863 T T T

Optimized 6 × 6 Au (111) surface structure on which two cyanides are adsorbed

1.00000000000000
 8.6514000000000006 -14.9846643566009998 0.0000000000000000
 8.6514000000000006 14.9846643566009998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 34.7092000000000027

Au C N

108 2 2

Selective dynamics

Direct

0.0014312958774886 0.0011268173231904 0.1379718417711152 T T T
 0.1111099999999965 0.0555599999999998 0.067839999999968 F F F
 0.5555599999999998 0.6111099999999965 0.0000000000000000 F F F
 0.0555599999999998 0.1111099999999965 0.0000000000000000 F F F
 0.1672031281062566 0.9996372366702035 0.1384887683947382 T T T
 0.2777799999999999 0.0555599999999998 0.067839999999968 F F F
 0.2222200000000001 0.1111099999999965 0.0000000000000000 F F F
 0.3333905318627013 0.9995221888972059 0.1375981312701340 T T T
 0.4444400000000002 0.0555599999999998 0.067839999999968 F F F
 0.3888900000000035 0.1111099999999965 0.0000000000000000 F F F
 0.4998408532209839 -0.0001775152219906 0.1376477657018834 T T T

0.6111099999999965 0.0555599999999998 0.0678399999999968 F F F
 0.5555599999999998 0.1111099999999965 0.0000000000000000 F F F
 0.7777799999999999 0.0555599999999998 0.0678399999999968 F F F
 0.4444400000000002 0.2222000000000001 0.0678399999999968 F F F
 0.7222200000000001 0.1111099999999965 0.0000000000000000 F F F
 0.8888900000000035 0.4444400000000002 0.0000000000000000 F F F
 0.9444400000000002 0.0555599999999998 0.0678399999999968 F F F
 0.8888900000000035 0.1111099999999965 0.0000000000000000 F F F
 0.0000185173521726 0.1670354128458094 0.1379464489196065 T T T
 0.0555599999999998 0.2777799999999999 0.0000000000000000 F F F
 0.1654448930624312 0.1649059659891511 0.1379858412955931 T T T
 0.2777799999999999 0.2222000000000001 0.0678399999999968 F F F
 0.2222200000000001 0.2777799999999999 0.0000000000000000 F F F
 0.6671249626791113 0.0015022631889941 0.1381422387759524 T T T
 0.1111099999999965 0.2222200000000001 0.0678399999999968 F F F
 0.8341425612992254 0.0018063272672131 0.1379905512669756 T T T
 0.6111099999999965 0.2222200000000001 0.0678399999999968 F F F
 0.7222200000000001 0.2777799999999999 0.0000000000000000 F F F
 0.7777799999999999 0.2222200000000001 0.0678399999999968 F F F
 0.8335847354841965 0.1672498150305456 0.1376729163983044 T T T
 0.9444400000000002 0.2222200000000001 0.0678399999999968 F F F
 0.1111099999999965 0.3888900000000035 0.0678399999999968 F F F
 0.9995061766075268 0.333008157833289 0.1379782798340102 T T T
 0.2777799999999999 0.3888900000000035 0.0678399999999968 F F F
 0.0555599999999998 0.4444400000000002 0.0000000000000000 F F F
 0.8888900000000035 0.2777799999999999 0.0000000000000000 F F F
 0.5555599999999998 0.2777799999999999 0.0000000000000000 F F F
 0.6665124509173708 0.1663624348841551 0.1374410139656556 T T T
 0.3327737500433959 0.1650759489109485 0.1380662467590485 T T T
 0.5555599999999998 0.4444400000000002 0.0000000000000000 F F F
 0.1648067035494300 0.3322398020004982 0.1380353594097614 T T T
 0.2222200000000001 0.4444400000000002 0.0000000000000000 F F F
 0.3286297320255861 0.3290790132845124 0.1370951858214699 T T T
 0.4444400000000002 0.3888900000000035 0.0678399999999968 F F F
 0.3888900000000035 0.4444400000000002 0.0000000000000000 F F F
 0.5001313706536519 0.3297331319347775 0.1369935673775702 T T T
 0.3888900000000035 0.2777799999999999 0.0000000000000000 F F F
 0.6671983996253302 0.3320376284981286 0.1379458032742086 T T T

0.7777799999999999 0.3888900000000035 0.0678399999999968 F F F
 0.7222200000000001 0.4444400000000002 0.0000000000000000 F F F
 0.4993298833261792 0.1649994706419139 0.1382673444029642 T T T
 0.9444400000000002 0.3888900000000035 0.0678399999999968 F F F
 0.8333436301255950 0.3326977931040642 0.1375905064740669 T T T
 0.0015863010635597 0.8339847348753647 0.1379477247679520 T T T
 0.6111099999999965 0.3888900000000035 0.0678399999999968 F F F
 0.0555599999999998 0.6111099999999965 0.0000000000000000 F F F
 0.1649879955573813 0.4995602650569781 0.1382895412614183 T T T
 0.2777799999999999 0.5555599999999998 0.0678399999999968 F F F
 0.2222200000000001 0.6111099999999965 0.0000000000000000 F F F
 0.3292374435307466 0.4993975808896792 0.1369936271654106 T T T
 0.4444400000000002 0.5555599999999998 0.0678399999999968 F F F
 0.3888900000000035 0.6111099999999965 0.0000000000000000 F F F
 0.6111099999999965 0.5555599999999998 0.0678399999999968 F F F
 0.6686024462419727 0.4983215906666401 0.1362683828016722 T T T
 0.7777799999999999 0.5555599999999998 0.0678399999999968 F F F
 0.7222200000000001 0.6111099999999965 0.0000000000000000 F F F
 0.8344056454306447 0.4991973282856724 0.1379732936077774 T T T
 0.9444400000000002 0.5555599999999998 0.0678399999999968 F F F
 0.8888900000000035 0.6111099999999965 0.0000000000000000 F F F
 0.001565455577064 0.6669836662696403 0.1381060423101884 T T T
 0.1111099999999965 0.7222200000000001 0.0678399999999968 F F F
 0.0555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.1666448113100981 0.6667558367043566 0.1377206543512781 T T T
 0.2777799999999999 0.7222200000000001 0.0678399999999968 F F F
 0.2222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.3322471730409043 0.6669747689319923 0.1380352132201524 T T T
 0.4444400000000002 0.7222200000000001 0.0678399999999968 F F F
 0.0001961809580373 0.4999210577637307 0.1375216429135441 T T T
 0.3888900000000035 0.7777799999999999 0.0000000000000000 F F F
 0.4983259709740867 0.6682961701337927 0.1359888458199692 T T T
 0.4969821709251407 0.4970808245318060 0.1380212221400156 T T T
 0.7222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.7777799999999999 0.7222200000000001 0.0678399999999968 F F F
 0.6111099999999965 0.7222200000000001 0.0678399999999968 F F F
 0.8370835013282956 0.6664300763893592 0.1370144803384216 T T T
 0.9444400000000002 0.7222200000000001 0.0678399999999968 F F F

0.8888900000000035 0.7777799999999999 0.0000000000000000 F F F
 0.111109999999965 0.8888900000000035 0.067839999999968 F F F
 0.0555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.1672172601163894 0.8334556554447888 0.1376022471367112 T T T
 0.2777799999999999 0.8888900000000035 0.067839999999968 F F F
 0.3331523865874625 0.8333094376423469 0.1383119502048955 T T T
 0.5555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.2222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.3888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.4444400000000002 0.8888900000000035 0.067839999999968 F F F
 0.8378808309600370 0.8385108217950723 0.1371509956176271 T T T
 0.7222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.7777799999999999 0.8888900000000035 0.067839999999968 F F F
 0.6670654248788681 0.8377297450901374 0.1371216056601231 T T T
 0.9444400000000002 0.8888900000000035 0.067839999999968 F F F
 0.5555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.6111099999999965 0.8888900000000035 0.067839999999968 F F F
 0.4995129777554696 0.8342047818675394 0.1380534688467359 T T T
 0.8888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.6705244214465689 0.6707513968394455 0.1385327704877729 T T T
 0.1111099999999965 0.5555599999999998 0.067839999999968 F F F
 0.4798005996025579 0.4804892003472009 0.1957800841444691 T T T
 0.6910987576792833 0.6914703540991202 0.1960335377972043 T T T
 0.4644954193260643 0.4653980645050338 0.2287340651449743 T T T
 0.7092512714381449 0.7103772212566920 0.2285739430077150 T T T

Optimized 6 × 6 Au (111) surface structure on which three cyanides are adsorbed

1.00000000000000
 8.651400000000006 -14.9846643566009998 0.0000000000000000
 8.651400000000006 14.9846643566009998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 34.709200000000027

Au C N

108 3 3

Selective dynamics

Direct

0.0014996102612577 0.0011957909485980 0.1381264894383625 T T T
 0.111109999999965 0.0555599999999998 0.067839999999968 F F F
 0.5555599999999998 0.611109999999965 0.0000000000000000 F F F

0.0555599999999998 0.1111099999999965 0.0000000000000000 F F F
 0.1668218066321477 0.9997311622427976 0.1383721236997504 T T T
 0.2777799999999999 0.0555599999999998 0.0678399999999968 F F F
 0.2222200000000001 0.1111099999999965 0.0000000000000000 F F F
 0.3328775366589674 -0.0003597043864493 0.1383646274781416 T T T
 0.4444400000000002 0.0555599999999998 0.0678399999999968 F F F
 0.3888900000000035 0.1111099999999965 0.0000000000000000 F F F
 0.4995790628262080 0.0010304246437202 0.1381300726266527 T T T
 0.6111099999999965 0.0555599999999998 0.0678399999999968 F F F
 0.5555599999999998 0.1111099999999965 0.0000000000000000 F F F
 0.7777799999999999 0.0555599999999998 0.0678399999999968 F F F
 0.4444400000000002 0.2222200000000001 0.0678399999999968 F F F
 0.7222200000000001 0.1111099999999965 0.0000000000000000 F F F
 0.8888900000000035 0.4444400000000002 0.0000000000000000 F F F
 0.9444400000000002 0.0555599999999998 0.0678399999999968 F F F
 0.8888900000000035 0.1111099999999965 0.0000000000000000 F F F
 -0.0003113907424899 0.1672864214546378 0.1380005939278064 T T T
 0.0555599999999998 0.2777799999999999 0.0000000000000000 F F F
 0.1650974358529204 0.1650437671456823 0.1380943710452225 T T T
 0.2777799999999999 0.2222200000000001 0.0678399999999968 F F F
 0.2222200000000001 0.2777799999999999 0.0000000000000000 F F F
 0.6674026851484846 0.0020422545322014 0.1381467298243851 T T T
 0.1111099999999965 0.2222200000000001 0.0678399999999968 F F F
 0.8348003404214173 0.0022517925403294 0.1381940520196879 T T T
 0.6111099999999965 0.2222200000000001 0.0678399999999968 F F F
 0.7222200000000001 0.2777799999999999 0.0000000000000000 F F F
 0.7777799999999999 0.2222200000000001 0.0678399999999968 F F F
 0.8335958340234495 0.1672555726564944 0.1380475355737802 T T T
 0.9444400000000002 0.2222200000000001 0.0678399999999968 F F F
 0.1111099999999965 0.3888900000000035 0.0678399999999968 F F F
 0.9995058429556476 0.3332308716137265 0.1380693580159622 T T T
 0.2777799999999999 0.3888900000000035 0.0678399999999968 F F F
 0.0555599999999998 0.4444400000000002 0.0000000000000000 F F F
 0.8888900000000035 0.2777799999999999 0.0000000000000000 F F F
 0.5555599999999998 0.2777799999999999 0.0000000000000000 F F F
 0.6670793487933560 0.1667524992781056 0.1379709666160121 T T T
 0.3324672681452964 0.1650245556871374 0.1380525907697888 T T T
 0.5555599999999998 0.4444400000000002 0.0000000000000000 F F F

0.1640282356739086 0.3317575079264884 0.1381692864200340 T T T
 0.2222200000000001 0.4444400000000002 0.0000000000000000 F F F
 0.3282745015089270 0.3286136115797165 0.1372337405581217 T T T
 0.4444400000000002 0.3888900000000035 0.067839999999968 F F F
 0.3888900000000035 0.4444400000000002 0.0000000000000000 F F F
 0.5004088147925482 0.3283882561178044 0.1371981963026285 T T T
 0.3888900000000035 0.2777799999999999 0.0000000000000000 F F F
 0.6676711423417270 0.3314942730017025 0.1382238022593997 T T T
 0.7777799999999999 0.3888900000000035 0.067839999999968 F F F
 0.7222200000000001 0.4444400000000002 0.0000000000000000 F F F
 0.4997753004188287 0.1648326154254711 0.1380895195210308 T T T
 0.9444400000000002 0.3888900000000035 0.067839999999968 F F F
 0.8335430004640303 0.3329643008249840 0.1380731586906416 T T T
 0.0015897825503421 0.8340111130744073 0.1380487689670226 T T T
 0.6111099999999965 0.3888900000000035 0.067839999999968 F F F
 0.0555599999999998 0.6111099999999965 0.0000000000000000 F F F
 0.1645308192047948 0.4992843000233461 0.1381741966306624 T T T
 0.2777799999999999 0.5555599999999998 0.067839999999968 F F F
 0.2222200000000001 0.6111099999999965 0.0000000000000000 F F F
 0.3275576864082097 0.4965878640917901 0.1367116201831921 T T T
 0.4444400000000002 0.5555599999999998 0.067839999999968 F F F
 0.3888900000000035 0.6111099999999965 0.0000000000000000 F F F
 0.6111099999999965 0.5555599999999998 0.067839999999968 F F F
 0.6695186972693007 0.4965189366608318 0.1367936790396521 T T T
 0.7777799999999999 0.5555599999999998 0.067839999999968 F F F
 0.7222200000000001 0.6111099999999965 0.0000000000000000 F F F
 0.8348960888304630 0.4991015723453194 0.1382218370981632 T T T
 0.9444400000000002 0.5555599999999998 0.067839999999968 F F F
 0.8888900000000035 0.6111099999999965 0.0000000000000000 F F F
 0.0015396236884053 0.6666283900019678 0.1380868345487488 T T T
 0.1111099999999965 0.7222200000000001 0.067839999999968 F F F
 0.0555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.1656065707514824 0.6669943094559438 0.1381430003765801 T T T
 0.2777799999999999 0.7222200000000001 0.067839999999968 F F F
 0.2222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.3285187371514774 0.6662130359588789 0.1371652764945472 T T T
 0.4444400000000002 0.7222200000000001 0.067839999999968 F F F
 -0.0001545517814286 0.4995424529822577 0.1380642044022102 T T T

0.3888900000000035 0.7777799999999999 0.0000000000000000 F F F
 0.4977659572868055 0.6686813105185782 0.1374569463876315 T T T
 0.4975734451023959 0.4943870217695165 0.1375241347027796 T T T
 0.7222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.7777799999999999 0.7222200000000001 0.0678399999999968 F F F
 0.6111099999999965 0.7222200000000001 0.0678399999999968 F F F
 0.8380883860026507 0.6662280745354475 0.1372216620044550 T T T
 0.9444400000000002 0.7222200000000001 0.0678399999999968 F F F
 0.8888900000000035 0.7777799999999999 0.0000000000000000 F F F
 0.1111099999999965 0.8888900000000035 0.0678399999999968 F F F
 0.0555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.1666498805353004 0.8332928016745657 0.1383616558904515 T T T
 0.2777799999999999 0.8888900000000035 0.0678399999999968 F F F
 0.3326244526267656 0.8341034847782989 0.1381878079651828 T T T
 0.5555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.2222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.3888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.4444400000000002 0.8888900000000035 0.0678399999999968 F F F
 0.8380064355508949 0.8384261868142691 0.1372430003603831 T T T
 0.7222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.7777799999999999 0.8888900000000035 0.0678399999999968 F F F
 0.6700473999974182 0.8392331116366176 0.1366525947424605 T T T
 0.9444400000000002 0.8888900000000035 0.0678399999999968 F F F
 0.5555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.6111099999999965 0.8888900000000035 0.0678399999999968 F F F
 0.5006715766262786 0.8383368852782471 0.1372262305897245 T T T
 0.8888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.6714574583709010 0.6681537949237778 0.1371948728816889 T T T
 0.1111099999999965 0.5555599999999998 0.0678399999999968 F F F
 0.4859509550868225 0.4707944702823477 0.1949378741929681 T T T
 0.6998003340527692 0.6868551633524584 0.1941805158509190 T T T
 0.4836796992073408 0.6859795531833484 0.1942842081742986 T T T
 0.4744706951209060 0.4480092220964747 0.2273110562787015 T T T
 0.7254191533606791 0.7024889184367790 0.2261357439501244 T T T
 0.4707561077875014 0.7000641793942851 0.2260647536768320 T T T

Optimized structure of methanol interacting with the cyanide adsorbed on the Au surface

1.00000000000000

8.6514000000000006 -14.9846643566009998 0.0000000000000000
 8.6514000000000006 14.9846643566009998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 34.7092000000000027

Au C H N O

108 2 4 1 1

Selective dynamics

Direct

0.0000115677172696 -0.0000453703371044 0.1373009286735087 T T T
 0.1111099999999965 0.0555599999999998 0.0678399999999968 F F F
 0.5555599999999998 0.6111099999999965 0.0000000000000000 F F F
 0.0555599999999998 0.1111099999999965 0.0000000000000000 F F F
 0.1667230236652333 -0.0002823194908575 0.1376368802245406 T T T
 0.2777799999999999 0.0555599999999998 0.0678399999999968 F F F
 0.2222200000000001 0.1111099999999965 0.0000000000000000 F F F
 0.3332724842515840 -0.0001056784782685 0.1376498564762877 T T T
 0.4444400000000002 0.0555599999999998 0.0678399999999968 F F F
 0.3888900000000035 0.1111099999999965 0.0000000000000000 F F F
 0.5000282254173972 0.0000611271526090 0.1372784411685310 T T T
 0.6111099999999965 0.0555599999999998 0.0678399999999968 F F F
 0.5555599999999998 0.1111099999999965 0.0000000000000000 F F F
 0.7777799999999999 0.0555599999999998 0.0678399999999968 F F F
 0.4444400000000002 0.2222200000000001 0.0678399999999968 F F F
 0.7222200000000001 0.1111099999999965 0.0000000000000000 F F F
 0.8888900000000035 0.4444400000000002 0.0000000000000000 F F F
 0.9444400000000002 0.0555599999999998 0.0678399999999968 F F F
 0.8888900000000035 0.1111099999999965 0.0000000000000000 F F F
 -0.0003482988122408 0.1664777460199790 0.1374554710820150 T T T
 0.0555599999999998 0.2777799999999999 0.0000000000000000 F F F
 0.1655904625302690 0.1653887567474693 0.1379248958191810 T T T
 0.2777799999999999 0.2222200000000001 0.0678399999999968 F F F
 0.3335057760994315 0.1666927330175230 0.1374113680153410 T T T
 0.6668807064470258 0.0003603548708633 0.1374481888134221 T T T
 0.1111099999999965 0.2222200000000001 0.0678399999999968 F F F
 0.8335287790960112 0.0003551445142732 0.1374529739522920 T T T
 0.6111099999999965 0.2222200000000001 0.0678399999999968 F F F
 0.7222200000000001 0.2777799999999999 0.0000000000000000 F F F
 0.7777799999999999 0.2222200000000001 0.0678399999999968 F F F
 0.8333537559994505 0.1666379445696387 0.1376699342195812 T T T

0.9444400000000002 0.222200000000001 0.067839999999968 F F F
 0.111109999999965 0.3888900000000035 0.067839999999968 F F F
 -0.0003337149807107 0.3331437106387493 0.1374685210264162 T T T
 0.277779999999999 0.3888900000000035 0.067839999999968 F F F
 0.0555599999999998 0.4444400000000002 0.0000000000000000 F F F
 0.8888900000000035 0.277779999999999 0.0000000000000000 F F F
 0.5555599999999998 0.277779999999999 0.0000000000000000 F F F
 0.6669506606283347 0.1664335251721340 0.1375795312299133 T T T
 0.8336326342920847 0.3329744354398795 0.1376110527494424 T T T
 0.5555599999999998 0.4444400000000002 0.0000000000000000 F F F
 0.1650802677919180 0.3324829359263083 0.1378320031863939 T T T
 0.2222200000000001 0.4444400000000002 0.0000000000000000 F F F
 0.3306379210170999 0.3313296636476646 0.1366396913666242 T T T
 0.4444400000000002 0.3888900000000035 0.067839999999968 F F F
 0.3888900000000035 0.4444400000000002 0.0000000000000000 F F F
 0.5008377594916428 0.3318740512379731 0.1366958120526444 T T T
 0.3888900000000035 0.277779999999999 0.0000000000000000 F F F
 0.6674138822541413 0.3324931848568672 0.1378750133078877 T T T
 0.777779999999999 0.3888900000000035 0.067839999999968 F F F
 0.7222200000000001 0.4444400000000002 0.0000000000000000 F F F
 0.5001798001296788 0.1657985496494636 0.1378098552541273 T T T
 0.9444400000000002 0.3888900000000035 0.067839999999968 F F F
 0.0002143313937167 0.8333443714870344 0.1376446590504606 T T T
 0.2222200000000001 0.277779999999999 0.0000000000000000 F F F
 0.111109999999965 0.5555599999999998 0.067839999999968 F F F
 0.3888900000000035 0.777779999999999 0.0000000000000000 F F F
 0.611109999999965 0.3888900000000035 0.067839999999968 F F F
 0.1655423653282304 0.5001336460488973 0.1380142157681069 T T T
 0.277779999999999 0.5555599999999998 0.067839999999968 F F F
 0.2222200000000001 0.611109999999965 0.0000000000000000 F F F
 0.3301677201080432 0.4993279499676971 0.1365025103905659 T T T
 0.4444400000000002 0.5555599999999998 0.067839999999968 F F F
 0.3888900000000035 0.611109999999965 0.0000000000000000 F F F
 0.611109999999965 0.5555599999999998 0.067839999999968 F F F
 0.6690296991497859 0.4995609432138668 0.1366832200500877 T T T
 0.777779999999999 0.5555599999999998 0.067839999999968 F F F
 0.5008222926317714 0.6699991266978270 0.1365311730445393 T T T
 0.7222200000000001 0.611109999999965 0.0000000000000000 F F F

0.9444400000000002 0.5555599999999998 0.0678399999999968 F F F
 0.8888900000000035 0.6111099999999965 0.0000000000000000 F F F
 0.000240883251406 0.6667982495916620 0.1374996757700580 T T T
 0.1111099999999965 0.7222200000000001 0.0678399999999968 F F F
 0.0555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.1667410644812898 0.6668008214450483 0.1376365382338048 T T T
 0.2777799999999999 0.7222200000000001 0.0678399999999968 F F F
 0.2222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.3333359955146931 0.667048311206537 0.1373742907003815 T T T
 0.4444400000000002 0.7222200000000001 0.0678399999999968 F F F
 0.0000228676884372 0.5000270729478478 0.1373056995174099 T T T
 0.8343295819709423 0.4996401433203663 0.1379449154775843 T T T
 0.5001210738853558 0.5000694985759622 0.1389463650709528 T T T
 0.0555599999999998 0.6111099999999965 0.0000000000000000 F F F
 0.8888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.669380503398714 0.6695565764154233 0.1364367377562462 T T T
 0.7777799999999999 0.7222200000000001 0.0678399999999968 F F F
 0.6111099999999965 0.7222200000000001 0.0678399999999968 F F F
 0.8339625575320897 0.6668202593182890 0.1375152031668280 T T T
 0.9444400000000002 0.7222200000000001 0.0678399999999968 F F F
 0.8888900000000035 0.7777799999999999 0.0000000000000000 F F F
 0.1111099999999965 0.8888900000000035 0.0678399999999968 F F F
 0.5555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.1667349982177566 0.833339402197208 0.1372974414519041 T T T
 0.2777799999999999 0.8888900000000035 0.0678399999999968 F F F
 0.3332998233436921 0.8334033724979573 0.1376918228275213 T T T
 0.0555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.2222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.5001823775047353 0.8346417742879766 0.1380297827889075 T T T
 0.7222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.5555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.9444400000000002 0.8888900000000035 0.0678399999999968 F F F
 0.6675820474261442 0.8349215674897111 0.1378036707823569 T T T
 0.6111099999999965 0.8888900000000035 0.0678399999999968 F F F
 0.7222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.8346332498325877 0.8344464853685319 0.1380167342786601 T T T
 0.4444400000000002 0.8888900000000035 0.0678399999999968 F F F
 0.3888900000000035 0.9444400000000002 0.0000000000000000 F F F

0.7777799999999999 0.8888900000000035 0.0678399999999968 F F F
 0.5016730789741870 0.5191249683266046 0.1968196533507118 T T T
 0.4804653748072366 0.3889504830836254 0.3098841463149967 T T T
 0.4910874729518862 0.3389563384933841 0.3247467702987663 T T T
 0.4167720345124449 0.3820618409308286 0.3202183305981590 T T T
 0.5350656676465049 0.4560518640173538 0.3178545047964996 T T T
 0.4834287042333743 0.4249913788661255 0.2562920787772608 T T T
 0.5023209735074735 0.5302354572821363 0.2302106656460574 T T T
 0.4787853769667192 0.3727247779204437 0.2695978020571103 T T T

Optimized structure of methanol interacting with two cyanides adsorbed on the Au surface

1.000000000000000
 8.6514000000000006 -14.9846643566009998 0.0000000000000000
 8.6514000000000006 14.9846643566009998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 34.7092000000000027
 Au C H N O
 108 3 4 2 1

Selective dynamics

Direct

0.0015141039632116 0.0015764154842569 0.1380567551252833 T T T
 0.1127729945390001 0.0591870608259981 0.0678895363920020 F F F
 0.5572229945390035 0.6147370608260019 0.0000495363919981 F F F
 0.0572229945390035 0.1147370608260019 0.0000495363919981 F F F
 0.1686064242232037 0.0013154130261940 0.1380911347160901 T T T
 0.2794429945389965 0.0591870608259981 0.0678895363920020 F F F
 0.2238829945389966 0.1147370608260019 0.0000495363919981 F F F
 0.3352338611386868 0.0009684959266684 0.1382576771388452 T T T
 0.4461029945389967 0.0591870608259981 0.0678895363920020 F F F
 0.3905529945390001 0.1147370608260019 0.0000495363919981 F F F
 0.5019166203713109 0.0019161918889033 0.1380052682917128 T T T
 0.6127729945390001 0.0591870608259981 0.0678895363920020 F F F
 0.5572229945390035 0.1147370608260019 0.0000495363919981 F F F
 0.7794429945389965 0.0591870608259981 0.0678895363920020 F F F
 0.4461029945389967 0.2258470608259984 0.0678895363920020 F F F
 0.7238829945389966 0.1147370608260019 0.0000495363919981 F F F
 0.8905529945390001 0.4480670608259985 0.0000495363919981 F F F
 0.9461029945389967 0.0591870608259981 0.0678895363920020 F F F
 0.8905529945390001 0.1147370608260019 0.0000495363919981 F F F

0.0003817576358106 0.1683931893191052 0.1380689104561350 T T T
 0.0572229945390035 0.2814070608259982 0.0000495363919981 F F F
 0.1644577968567612 0.1650902642839719 0.1369890662463713 T T T
 0.2794429945389965 0.2258470608259984 0.0678895363920020 F F F
 0.3361633109546966 0.1662158820989578 0.1370300493883241 T T T
 0.6688537519393052 0.0027739575868527 0.1380529177987488 T T T
 0.1127729945390001 0.2258470608259984 0.0678895363920020 F F F
 0.8354412261765081 0.0028659321425740 0.1380302795104787 T T T
 0.6127729945390001 0.2258470608259984 0.0678895363920020 F F F
 0.7238829945389966 0.2814070608259982 0.0000495363919981 F F F
 0.7794429945389965 0.2258470608259984 0.0678895363920020 F F F
 0.8347307295874979 0.1687274684615322 0.1380903847543281 T T T
 0.9461029945389967 0.2258470608259984 0.0678895363920020 F F F
 0.1127729945390001 0.3925170608260018 0.0678895363920020 F F F
 0.0007837959275038 0.3353571515918587 0.1382333468695104 T T T
 0.2794429945389965 0.3925170608260018 0.0678895363920020 F F F
 0.0572229945390035 0.4480670608259985 0.0000495363919981 F F F
 0.8905529945390001 0.2814070608259982 0.0000495363919981 F F F
 0.5572229945390035 0.2814070608259982 0.0000495363919981 F F F
 0.6687188205092838 0.1685160130596726 0.1380372457334951 T T T
 0.8353637417475593 0.3351378342280613 0.1379655589941443 T T T
 0.5572229945390035 0.4480670608259985 0.0000495363919981 F F F
 0.1649186170303599 0.3349074262602026 0.1371250815442785 T T T
 0.2238829945389966 0.4480670608259985 0.0000495363919981 F F F
 0.3332467358375442 0.3330546500099432 0.1388333295920288 T T T
 0.4461029945389967 0.3925170608260018 0.0678895363920020 F F F
 0.3905529945390001 0.4480670608259985 0.0000495363919981 F F F
 0.5040690004867591 0.3335955320893795 0.1369047505062395 T T T
 0.3905529945390001 0.2814070608259982 0.0000495363919981 F F F
 0.6698229973158641 0.3348662772357702 0.1380659365750354 T T T
 0.7794429945389965 0.3925170608260018 0.0678895363920020 F F F
 0.7238829945389966 0.4480670608259985 0.0000495363919981 F F F
 0.5024565453439835 0.1676403182045242 0.1381381360694578 T T T
 0.9461029945389967 0.3925170608260018 0.0678895363920020 F F F
 0.0020954727631950 0.8352115633302054 0.1381091665596849 T T T
 0.2238829945389966 0.2814070608259982 0.0000495363919981 F F F
 0.1127729945390001 0.5591870608259981 0.0678895363920020 F F F
 0.3905529945390001 0.7814070608259982 0.0000495363919981 F F F

0.6127729945390001 0.3925170608260018 0.0678895363920020 F F F
 0.1677163060250842 0.5024023117825607 0.1380612578698287 T T T
 0.2794429945389965 0.5591870608259981 0.0678895363920020 F F F
 0.2238829945389966 0.6147370608260019 0.0000495363919981 F F F
 0.3337016430438054 0.5040695180712967 0.1360232847502512 T T T
 0.4461029945389967 0.5591870608259981 0.0678895363920020 F F F
 0.3905529945390001 0.6147370608260019 0.0000495363919981 F F F
 0.6127729945390001 0.5591870608259981 0.0678895363920020 F F F
 0.6716927905709850 0.5013582280999603 0.1370832811513196 T T T
 0.7794429945389965 0.5591870608259981 0.0678895363920020 F F F
 0.5032419527073020 0.6735921772505183 0.1371598560088273 T T T
 0.7238829945389966 0.6147370608260019 0.0000495363919981 F F F
 0.9461029945389967 0.5591870608259981 0.0678895363920020 F F F
 0.8905529945390001 0.6147370608260019 0.0000495363919981 F F F
 0.0020538382539643 0.6687523536274507 0.1380042720379321 T T T
 0.1127729945390001 0.7258470608259984 0.0678895363920020 F F F
 0.0572229945390035 0.7814070608259982 0.0000495363919981 F F F
 0.1683224498742603 0.6687716620092867 0.1380319085189223 T T T
 0.2794429945389965 0.7258470608259984 0.0678895363920020 F F F
 0.2238829945389966 0.7814070608259982 0.0000495363919981 F F F
 0.3350289379433334 0.6698570199528195 0.1380511088481242 T T T
 0.4461029945389967 0.7258470608259984 0.0678895363920020 F F F
 0.0017414870641219 0.5020097686446967 0.1380108228178008 T T T
 0.8365786341628518 0.5023022969608559 0.1384278692207267 T T T
 0.5055098371315707 0.5062069492445088 0.1382425740156894 T T T
 0.0572229945390035 0.6147370608260019 0.0000495363919981 F F F
 0.8905529945390001 0.9480670608259985 0.0000495363919981 F F F
 0.6730603284022190 0.6735295765545700 0.1370422881812681 T T T
 0.7794429945389965 0.7258470608259984 0.0678895363920020 F F F
 0.6127729945390001 0.7258470608259984 0.0678895363920020 F F F
 0.8362661058935309 0.6693356533998710 0.1380392485248419 T T T
 0.9461029945389967 0.7258470608259984 0.0678895363920020 F F F
 0.8905529945390001 0.7814070608259982 0.0000495363919981 F F F
 0.1127729945390001 0.8925170608260018 0.0678895363920020 F F F
 0.5572229945390035 0.7814070608259982 0.0000495363919981 F F F
 0.1683174709094606 0.8351497186004577 0.1379851499713107 T T T
 0.2794429945389965 0.8925170608260018 0.0678895363920020 F F F
 0.3350191808984371 0.8353378550000549 0.1379862958701969 T T T

0.0572229945390035 0.9480670608259985 0.0000495363919981 F F F
 0.2238829945389966 0.9480670608259985 0.0000495363919981 F F F
 0.5023756917021812 0.8371800890149660 0.1383527062718845 T T T
 0.7238829945389966 0.7814070608259982 0.0000495363919981 F F F
 0.5572229945390035 0.9480670608259985 0.0000495363919981 F F F
 0.9461029945389967 0.8925170608260018 0.0678895363920020 F F F
 0.6699964069292405 0.8377154305160223 0.1382631041118848 T T T
 0.6127729945390001 0.8925170608260018 0.0678895363920020 F F F
 0.7238829945389966 0.9480670608259985 0.0000495363919981 F F F
 0.8368362575804803 0.8370012689986386 0.1380868755315291 T T T
 0.4461029945389967 0.8925170608260018 0.0678895363920020 F F F
 0.3905529945390001 0.9480670608259985 0.0000495363919981 F F F
 0.7794429945389965 0.8925170608260018 0.0678895363920020 F F F
 0.5143729285252364 0.5187855109248114 0.1963749568814348 T T T
 0.4886523788832973 0.3827010195602573 0.3078779525304888 T T T
 0.3008331260719347 0.3144950914474555 0.1956531344865853 T T T
 0.4944474101247082 0.3331411367397193 0.3254631637669321 T T T
 0.4184479121972923 0.3668438348345533 0.3080471388604163 T T T
 0.5298728603914357 0.4492518319968249 0.3210289833771823 T T T
 0.5170644804683566 0.4267511326765426 0.2551852637629765 T T T
 0.5228252231453393 0.5260401953101665 0.2299454164603868 T T T
 0.2748522739525026 0.2986065070014942 0.2275613956390340 T T T
 0.5181597146789049 0.3788227854032623 0.2700583688394046 T T T

Optimized structure of methanol interacting with three cyanides adsorbed on the Au surface

1.00000000000000
 8.651400000000006 -14.9846643566009998 0.0000000000000000
 8.651400000000006 14.9846643566009998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 34.7092000000000027

Au C H N O

108 4 4 3 1

Selective dynamics

Direct

0.0010774313256225 0.0017518991803607 0.1384621076840025 T T T
 0.1127729945390001 0.0591870608259981 0.0678895363920020 F F F
 0.5572229945390035 0.6147370608260019 0.0000495363919981 F F F
 0.0572229945390035 0.1147370608260019 0.0000495363919981 F F F
 0.1678467022742843 0.0009929712349355 0.1385366683669246 T T T

0.2794429945389965 0.0591870608259981 0.0678895363920020 F F F
 0.2238829945389966 0.1147370608260019 0.0000495363919981 F F F
 0.3341592107228176 0.0001539987338619 0.1386126429972802 T T T
 0.4461029945389967 0.0591870608259981 0.0678895363920020 F F F
 0.3905529945390001 0.1147370608260019 0.0000495363919981 F F F
 0.5020558628068303 0.0011829483978092 0.1382035405607832 T T T
 0.6127729945390001 0.0591870608259981 0.0678895363920020 F F F
 0.5572229945390035 0.1147370608260019 0.0000495363919981 F F F
 0.7794429945389965 0.0591870608259981 0.0678895363920020 F F F
 0.4461029945389967 0.2258470608259984 0.0678895363920020 F F F
 0.7238829945389966 0.1147370608260019 0.0000495363919981 F F F
 0.8905529945390001 0.4480670608259985 0.0000495363919981 F F F
 0.9461029945389967 0.0591870608259981 0.0678895363920020 F F F
 0.8905529945390001 0.1147370608260019 0.0000495363919981 F F F
 -0.0001538513196569 0.1683558189284261 0.1380397640063487 T T T
 0.0572229945390035 0.2814070608259982 0.0000495363919981 F F F
 0.1633250450017119 0.1648007983021272 0.1374928452954418 T T T
 0.2794429945389965 0.2258470608259984 0.0678895363920020 F F F
 0.3330338695214288 0.1649717048567680 0.1357961489646951 T T T
 0.6695041138386482 0.0031285316153784 0.1382801652781784 T T T
 0.1127729945390001 0.2258470608259984 0.0678895363920020 F F F
 0.8353378954496573 0.0029021082481383 0.1383388414642799 T T T
 0.6127729945390001 0.2258470608259984 0.0678895363920020 F F F
 0.7238829945389966 0.2814070608259982 0.0000495363919981 F F F
 0.7794429945389965 0.2258470608259984 0.0678895363920020 F F F
 0.8352016247623272 0.1692086802981292 0.1383449644964797 T T T
 0.9461029945389967 0.2258470608259984 0.0678895363920020 F F F
 0.1127729945390001 0.3925170608260018 0.0678895363920020 F F F
 0.0008100037178090 0.3359525634271693 0.1383033865830993 T T T
 0.2794429945389965 0.3925170608260018 0.0678895363920020 F F F
 0.0572229945390035 0.4480670608259985 0.0000495363919981 F F F
 0.8905529945390001 0.2814070608259982 0.0000495363919981 F F F
 0.5572229945390035 0.2814070608259982 0.0000495363919981 F F F
 0.6700545451953336 0.1686245579575864 0.1377432249228531 T T T
 0.8373220305828346 0.3365547156296148 0.1386450426194051 T T T
 0.5572229945390035 0.4480670608259985 0.0000495363919981 F F F
 0.1637217720160555 0.3351472129848907 0.1373356045665957 T T T
 0.2238829945389966 0.4480670608259985 0.0000495363919981 F F F

0.3312449297018296 0.3334629196115653 0.1379483991126799 T T T
 0.4461029945389967 0.3925170608260018 0.0678895363920020 F F F
 0.3905529945390001 0.4480670608259985 0.0000495363919981 F F F
 0.5049289034362830 0.3385561669572171 0.1382964948251223 T T T
 0.3905529945390001 0.2814070608259982 0.0000495363919981 F F F
 0.6757955997630678 0.3379665742892817 0.1369875566234709 T T T
 0.7794429945389965 0.3925170608260018 0.0678895363920020 F F F
 0.7238829945389966 0.4480670608259985 0.0000495363919981 F F F
 0.5016119997792157 0.1635631091395058 0.1374910280249520 T T T
 0.9461029945389967 0.3925170608260018 0.0678895363920020 F F F
 0.0030140023229461 0.8363485222348007 0.1382449394466078 T T T
 0.2238829945389966 0.2814070608259982 0.0000495363919981 F F F
 0.1127729945390001 0.5591870608259981 0.0678895363920020 F F F
 0.3905529945390001 0.7814070608259982 0.0000495363919981 F F F
 0.6127729945390001 0.3925170608260018 0.0678895363920020 F F F
 0.1678873835582622 0.5031484269518673 0.1382396712458328 T T T
 0.2794429945389965 0.5591870608259981 0.0678895363920020 F F F
 0.2238829945389966 0.6147370608260019 0.0000495363919981 F F F
 0.3333831616418130 0.5053014057670536 0.1365534721132115 T T T
 0.4461029945389967 0.5591870608259981 0.0678895363920020 F F F
 0.3905529945390001 0.6147370608260019 0.0000495363919981 F F F
 0.6127729945390001 0.5591870608259981 0.0678895363920020 F F F
 0.6748079317748878 0.5070174805767540 0.1362895158648705 T T T
 0.7794429945389965 0.5591870608259981 0.0678895363920020 F F F
 0.5036326102083428 0.6753690248343559 0.1371736684615908 T T T
 0.7238829945389966 0.6147370608260019 0.0000495363919981 F F F
 0.9461029945389967 0.5591870608259981 0.0678895363920020 F F F
 0.8905529945390001 0.6147370608260019 0.0000495363919981 F F F
 0.0031299227327873 0.6698464819773331 0.1380747416324482 T T T
 0.1127729945390001 0.7258470608259984 0.0678895363920020 F F F
 0.0572229945390035 0.7814070608259982 0.0000495363919981 F F F
 0.1688032840231224 0.6692580396609378 0.1381334658262730 T T T
 0.2794429945389965 0.7258470608259984 0.0678895363920020 F F F
 0.2238829945389966 0.7814070608259982 0.0000495363919981 F F F
 0.3353307498969593 0.6707963307076513 0.1383127378094394 T T T
 0.4461029945389967 0.7258470608259984 0.0678895363920020 F F F
 0.0029379929716163 0.5032829925737345 0.1383603038497062 T T T
 0.8386215599985553 0.5047568263189018 0.1387402504537015 T T T

0.5056256957981498 0.5099457207832148 0.1382040661383672 T T T
 0.0572229945390035 0.6147370608260019 0.0000495363919981 F F F
 0.8905529945390001 0.9480670608259985 0.0000495363919981 F F F
 0.6741390843693538 0.6756354191363050 0.1372978956032451 T T T
 0.7794429945389965 0.7258470608259984 0.0678895363920020 F F F
 0.6127729945390001 0.7258470608259984 0.0678895363920020 F F F
 0.8382926248733330 0.6716476328319885 0.1384794110333365 T T T
 0.9461029945389967 0.7258470608259984 0.0678895363920020 F F F
 0.8905529945390001 0.7814070608259982 0.0000495363919981 F F F
 0.1127729945390001 0.8925170608260018 0.0678895363920020 F F F
 0.5572229945390035 0.7814070608259982 0.0000495363919981 F F F
 0.1685500571862065 0.8352881683801767 0.1380566926574614 T T T
 0.2794429945389965 0.8925170608260018 0.0678895363920020 F F F
 0.3348103639904311 0.8354760922762238 0.1381794945146028 T T T
 0.0572229945390035 0.9480670608259985 0.0000495363919981 F F F
 0.2238829945389966 0.9480670608259985 0.0000495363919981 F F F
 0.5027456582318373 0.8379736531774933 0.1383318133940289 T T T
 0.7238829945389966 0.7814070608259982 0.0000495363919981 F F F
 0.5572229945390035 0.9480670608259985 0.0000495363919981 F F F
 0.9461029945389967 0.8925170608260018 0.0678895363920020 F F F
 0.6704416340089693 0.8384617828864104 0.1383566195975360 T T T
 0.6127729945390001 0.8925170608260018 0.0678895363920020 F F F
 0.7238829945389966 0.9480670608259985 0.0000495363919981 F F F
 0.8377611014620167 0.8382429585373138 0.1386774141585738 T T T
 0.4461029945389967 0.8925170608260018 0.0678895363920020 F F F
 0.3905529945390001 0.9480670608259985 0.0000495363919981 F F F
 0.7794429945389965 0.8925170608260018 0.0678895363920020 F F F
 0.5093191734545069 0.5162089996613954 0.1965841555805210 T T T
 0.4819024843528978 0.3936238526073028 0.3180211287812644 T T T
 0.2944495200597055 0.3137197215166876 0.1942566138149939 T T T
 0.5281971322336464 0.2889113253529370 0.1879662286874805 T T T
 0.4851228050577491 0.3413775292073771 0.3347070592287051 T T T
 0.4202689787085851 0.3940741958308182 0.3260621237608757 T T T
 0.5395830424851669 0.4590960628339153 0.3258070952749443 T T T
 0.4877682224561257 0.4240492484669274 0.2631774118459433 T T T
 0.5122847250006471 0.5197045922034301 0.2303278233017172 T T T
 0.2642394844133600 0.2983839736505279 0.2255095199871967 T T T
 0.5437483605237847 0.2534312694501162 0.2134378253575018 T T T

0.4826695630504024 0.3736447350061105 0.2784663468306839 T T T

Optimized structure of methylamine interacting with the cyanide adsorbed on the Au surface

1.00000000000000
8.6514000000000006 -14.9846643566009998 0.0000000000000000
8.6514000000000006 14.9846643566009998 0.0000000000000000
0.0000000000000000 0.0000000000000000 34.7092000000000027

Au C H N

108 2 5 2

Selective dynamics

Direct

-0.0000295372243188 -0.0000858898560427 0.1373042851706381 T T T
0.1111099999999965 0.0555599999999998 0.0678399999999968 F F F
0.5555599999999998 0.6111099999999965 0.0000000000000000 F F F
0.0555599999999998 0.1111099999999965 0.0000000000000000 F F F
0.1663639287466178 -0.0006750036739506 0.1375948324586972 T T T
0.2777799999999999 0.0555599999999998 0.0678399999999968 F F F
0.2222200000000001 0.1111099999999965 0.0000000000000000 F F F
0.3329856912459164 -0.0006803950272021 0.1375684339881056 T T T
0.4444400000000002 0.0555599999999998 0.0678399999999968 F F F
0.3888900000000035 0.1111099999999965 0.0000000000000000 F F F
0.4999843355591951 -0.0001910677790241 0.1373151473330363 T T T
0.6111099999999965 0.0555599999999998 0.0678399999999968 F F F
0.5555599999999998 0.1111099999999965 0.0000000000000000 F F F
0.7777799999999999 0.0555599999999998 0.0678399999999968 F F F
0.4444400000000002 0.2222200000000001 0.0678399999999968 F F F
0.7222200000000001 0.1111099999999965 0.0000000000000000 F F F
0.8888900000000035 0.4444400000000002 0.0000000000000000 F F F
0.9444400000000002 0.0555599999999998 0.0678399999999968 F F F
0.8888900000000035 0.1111099999999965 0.0000000000000000 F F F
-0.0004193233236177 0.1664273887328900 0.1374320470565317 T T T
0.0555599999999998 0.2777799999999999 0.0000000000000000 F F F
0.1653722120867603 0.1652246026671543 0.1379532603707196 T T T
0.2222200000000001 0.2777799999999999 0.0000000000000000 F F F
0.3328586255210227 0.1654919778757167 0.1375471161218745 T T T
0.6669348158537697 0.0003304777236260 0.1374079927368743 T T T
0.1111099999999965 0.2222200000000001 0.0678399999999968 F F F
0.8334976441369444 0.0003539787329250 0.1373887423738834 T T T

0.6111099999999965 0.2222200000000001 0.0678399999999968 F F F
 0.7222200000000001 0.2777799999999999 0.0000000000000000 F F F
 0.7777799999999999 0.2222200000000001 0.0678399999999968 F F F
 0.8333228516753153 0.1666532823587905 0.1377006809001133 T T T
 0.9444400000000002 0.2222200000000001 0.0678399999999968 F F F
 0.1111099999999965 0.3888900000000035 0.0678399999999968 F F F
 -0.0006495855435389 0.3328740684841948 0.1375263428209507 T T T
 0.2777799999999999 0.3888900000000035 0.0678399999999968 F F F
 0.0555599999999998 0.4444400000000002 0.0000000000000000 F F F
 0.8888900000000035 0.2777799999999999 0.0000000000000000 F F F
 0.5555599999999998 0.2777799999999999 0.0000000000000000 F F F
 0.6669709864308606 0.1663194259972068 0.1375530670537968 T T T
 0.8334948837847813 0.3329091572195749 0.1375883459925905 T T T
 0.5555599999999998 0.4444400000000002 0.0000000000000000 F F F
 0.1650381416742638 0.3323528973225058 0.1378544665709582 T T T
 0.2222200000000001 0.4444400000000002 0.0000000000000000 F F F
 0.3305040625287037 0.3303730105486941 0.1368478409169840 T T T
 0.4444400000000002 0.3888900000000035 0.0678399999999968 F F F
 0.3888900000000035 0.4444400000000002 0.0000000000000000 F F F
 0.5002409682154145 0.3309839826779850 0.1369426413448166 T T T
 0.3888900000000035 0.2777799999999999 0.0000000000000000 F F F
 0.6672612912294951 0.3323973133092896 0.1379066504902860 T T T
 0.7777799999999999 0.3888900000000035 0.0678399999999968 F F F
 0.7222200000000001 0.4444400000000002 0.0000000000000000 F F F
 0.4999858189042251 0.1653123433649597 0.1378968305693123 T T T
 0.9444400000000002 0.3888900000000035 0.0678399999999968 F F F
 0.0000563697980365 0.8332535711975768 0.1376730938903385 T T T
 0.2777799999999999 0.2222200000000001 0.0678399999999968 F F F
 0.1111099999999965 0.5555599999999998 0.0678399999999968 F F F
 0.3888900000000035 0.7777799999999999 0.0000000000000000 F F F
 0.6111099999999965 0.3888900000000035 0.0678399999999968 F F F
 0.1652937225820851 0.4995508933672317 0.1379279898143935 T T T
 0.2777799999999999 0.5555599999999998 0.0678399999999968 F F F
 0.2222200000000001 0.6111099999999965 0.0000000000000000 F F F
 0.3301259818715601 0.4987482508802904 0.1364474964308836 T T T
 0.4444400000000002 0.5555599999999998 0.0678399999999968 F F F
 0.3888900000000035 0.6111099999999965 0.0000000000000000 F F F
 0.6111099999999965 0.5555599999999998 0.0678399999999968 F F F

0.6684091731937654 0.4989376004047892 0.1365986848612826 T T T
 0.7777799999999999 0.5555599999999998 0.0678399999999968 F F F
 0.5006095096794970 0.6697769011130393 0.1364863942781730 T T T
 0.7222200000000001 0.6111099999999965 0.0000000000000000 F F F
 0.9444400000000002 0.5555599999999998 0.0678399999999968 F F F
 0.8888900000000035 0.6111099999999965 0.0000000000000000 F F F
 0.0000617978903045 0.6666895645125973 0.1376625607880976 T T T
 0.1111099999999965 0.7222200000000001 0.0678399999999968 F F F
 0.0555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.1666580510874574 0.6666952082629866 0.1376660757988131 T T T
 0.2777799999999999 0.7222200000000001 0.0678399999999968 F F F
 0.2222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.333092840795062 0.6666351770972955 0.1373821131785239 T T T
 0.4444400000000002 0.7222200000000001 0.0678399999999968 F F F
 0.0000122032921231 0.4999880597239674 0.1372983266275054 T T T
 0.8342236246704229 0.4994739816386179 0.1379216293027316 T T T
 0.4993606498004096 0.4986231424252467 0.1390510180999587 T T T
 0.0555599999999998 0.6111099999999965 0.0000000000000000 F F F
 0.8888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.6693984654006856 0.6696154454758398 0.1364389529729419 T T T
 0.7777799999999999 0.7222200000000001 0.0678399999999968 F F F
 0.6111099999999965 0.7222200000000001 0.0678399999999968 F F F
 0.8337300831697029 0.6665722330087871 0.1374715133079629 T T T
 0.9444400000000002 0.7222200000000001 0.0678399999999968 F F F
 0.8888900000000035 0.7777799999999999 0.0000000000000000 F F F
 0.1111099999999965 0.8888900000000035 0.0678399999999968 F F F
 0.5555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.1665319359851074 0.8331202022595278 0.1373419178963703 T T T
 0.2777799999999999 0.8888900000000035 0.0678399999999968 F F F
 0.3332575641343998 0.8332139516309792 0.1376635984084491 T T T
 0.0555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.2222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.5002482039297514 0.8344266511281782 0.1379613784253498 T T T
 0.7222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.5555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.9444400000000002 0.8888900000000035 0.0678399999999968 F F F
 0.6675195873566401 0.8348935135030495 0.1379513199149889 T T T
 0.6111099999999965 0.8888900000000035 0.0678399999999968 F F F

0.7222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.8344793566613696 0.8345527513599968 0.1379566579377286 T T T
 0.4444400000000002 0.8888900000000035 0.0678399999999968 F F F
 0.3888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.7777799999999999 0.8888900000000035 0.0678399999999968 F F F
 0.5055138660087670 0.5297191656261886 0.1959096080532841 T T T
 0.4836786066055176 0.3896472339456536 0.3110496102890747 T T T
 0.4731869286806112 0.4234525964494472 0.2552727975498487 T T T
 0.4959546103079090 0.3408285665567868 0.3259497318513288 T T T
 0.4176973131397251 0.3775496923355820 0.3200957855188349 T T T
 0.5336832776808672 0.4569694155109071 0.3213276575287576 T T T
 0.5441958570432981 0.3877499812120926 0.2601302913736063 T T T
 0.5089660188151555 0.5509364596410093 0.2282983076848321 T T T
 0.4839671617856321 0.3778941067861922 0.2694283068168326 T T T

Optimized structure of methylamine interacting with two cyanides adsorbed on the Au surface

1.00000000000000
 8.651400000000006 -14.9846643566009998 0.0000000000000000
 8.651400000000006 14.9846643566009998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 34.7092000000000027

Au C H N

108 3 5 3

Selective dynamics

Direct

-0.0000195103361782 -0.0001214617043042 0.1374790029739593 T T T
 0.1111099999999965 0.0555599999999998 0.0678399999999968 F F F
 0.5555599999999998 0.6111099999999965 0.0000000000000000 F F F
 0.0555599999999998 0.1111099999999965 0.0000000000000000 F F F
 0.1667032508749829 0.9999119968592799 0.1376495956231889 T T T
 0.2777799999999999 0.0555599999999998 0.0678399999999968 F F F
 0.2222200000000001 0.1111099999999965 0.0000000000000000 F F F
 0.3332801689186422 0.9998217687841570 0.1377156571387730 T T T
 0.4444400000000002 0.0555599999999998 0.0678399999999968 F F F
 0.3888900000000035 0.1111099999999965 0.0000000000000000 F F F
 0.4997098913994838 0.9994848107327614 0.1375966530791322 T T T
 0.6111099999999965 0.0555599999999998 0.0678399999999968 F F F
 0.5555599999999998 0.1111099999999965 0.0000000000000000 F F F
 0.7777799999999999 0.0555599999999998 0.0678399999999968 F F F

0.4444400000000002 0.222200000000001 0.067839999999968 F F F
 0.722200000000001 0.11109999999965 0.000000000000000 F F F
 0.8888900000000035 0.444440000000002 0.000000000000000 F F F
 0.9444400000000002 0.055599999999998 0.067839999999968 F F F
 0.8888900000000035 0.11109999999965 0.000000000000000 F F F
 0.9991711333946771 0.1656888425125879 0.1376996314429423 T T T
 0.055599999999998 0.277779999999999 0.000000000000000 F F F
 0.1649763196540898 0.1650271739695853 0.1380634382145698 T T T
 0.222200000000001 0.277779999999999 0.000000000000000 F F F
 0.3323872360077932 0.1650892645793252 0.1380000165056960 T T T
 0.666696274239448 0.0000808473818302 0.1373973815111178 T T T
 0.11109999999965 0.222200000000001 0.067839999999968 F F F
 0.8333675713000541 0.0001305181885443 0.1376940926318135 T T T
 0.611109999999965 0.222200000000001 0.067839999999968 F F F
 0.722200000000001 0.277779999999999 0.000000000000000 F F F
 0.777779999999999 0.222200000000001 0.067839999999968 F F F
 0.8332436746768691 0.166059283530510 0.1376961150893439 T T T
 0.9444400000000002 0.222200000000001 0.067839999999968 F F F
 0.111109999999965 0.3888900000000035 0.067839999999968 F F F
 0.9993575538233277 0.3318856389286833 0.1380577200569904 T T T
 0.277779999999999 0.3888900000000035 0.067839999999968 F F F
 0.055599999999998 0.4444400000000002 0.000000000000000 F F F
 0.8888900000000035 0.277779999999999 0.000000000000000 F F F
 0.555599999999998 0.277779999999999 0.000000000000000 F F F
 0.6667314478097510 0.1651478239919638 0.1381081095643047 T T T
 0.8341269617200628 0.3321301302767969 0.1380442833722347 T T T
 0.555599999999998 0.4444400000000002 0.000000000000000 F F F
 0.1647316482837146 0.3317707747683348 0.1380171344299823 T T T
 0.222200000000001 0.4444400000000002 0.000000000000000 F F F
 0.3289826573740489 0.3292138474720173 0.1371426824318035 T T T
 0.4444400000000002 0.3888900000000035 0.067839999999968 F F F
 0.3888900000000035 0.4444400000000002 0.000000000000000 F F F
 0.4981710576476140 0.3300916593524642 0.1362372869046570 T T T
 0.3888900000000035 0.277779999999999 0.000000000000000 F F F
 0.6670803896003411 0.3294712274554721 0.1369845258812770 T T T
 0.777779999999999 0.3888900000000035 0.067839999999968 F F F
 0.722200000000001 0.4444400000000002 0.000000000000000 F F F
 0.4995155031763700 0.1650403920753933 0.1379870033498700 T T T

0.9444400000000002 0.3888900000000035 0.067839999999968 F F F
 0.0017608048860463 0.8344613395206749 0.1380783290498261 T T T
 0.2777799999999999 0.222200000000001 0.067839999999968 F F F
 0.1111099999999965 0.5555599999999998 0.067839999999968 F F F
 0.3888900000000035 0.7777799999999999 0.0000000000000000 F F F
 0.6111099999999965 0.3888900000000035 0.067839999999968 F F F
 0.1650794451542826 0.4994879368231292 0.1379965213516587 T T T
 0.2777799999999999 0.5555599999999998 0.067839999999968 F F F
 0.222200000000001 0.6111099999999965 0.0000000000000000 F F F
 0.3280685415023024 0.4990241032585694 0.1367394721287906 T T T
 0.4444400000000002 0.5555599999999998 0.067839999999968 F F F
 0.3888900000000035 0.6111099999999965 0.0000000000000000 F F F
 0.6111099999999965 0.5555599999999998 0.067839999999968 F F F
 0.6712527545352406 0.5002440048208254 0.1384940989617853 T T T
 0.7777799999999999 0.5555599999999998 0.067839999999968 F F F
 0.5002757002473269 0.6704354433521335 0.1368779969787396 T T T
 0.722200000000001 0.6111099999999965 0.0000000000000000 F F F
 0.9444400000000002 0.5555599999999998 0.067839999999968 F F F
 0.8888900000000035 0.6111099999999965 0.0000000000000000 F F F
 0.0015538263926860 0.6674308761567045 0.1379472031114516 T T T
 0.1111099999999965 0.722200000000001 0.067839999999968 F F F
 0.0555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.1671275507100353 0.6671834050872150 0.1380360784750910 T T T
 0.2777799999999999 0.722200000000001 0.067839999999968 F F F
 0.222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.3326736791567174 0.6673231968395555 0.1380100859933703 T T T
 0.4444400000000002 0.722200000000001 0.067839999999968 F F F
 0.0015405412483545 0.4997291641904460 0.1380095043304697 T T T
 0.8382479106507577 0.4996198304097840 0.137017866552684 T T T
 0.4960358196523023 0.4977206280095892 0.1377838825498544 T T T
 0.0555599999999998 0.6111099999999965 0.0000000000000000 F F F
 0.8888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.6691551378813559 0.6705349103290965 0.1359690706934918 T T T
 0.7777799999999999 0.722200000000001 0.067839999999968 F F F
 0.6111099999999965 0.722200000000001 0.067839999999968 F F F
 0.8371657559860667 0.6705601237135813 0.1370053156821042 T T T
 0.9444400000000002 0.722200000000001 0.067839999999968 F F F
 0.8888900000000035 0.7777799999999999 0.0000000000000000 F F F

0.1111099999999965 0.8888900000000035 0.0678399999999968 F F F
 0.5555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.1674072002544018 0.8337275973439114 0.1375636163497826 T T T
 0.2777799999999999 0.8888900000000035 0.0678399999999968 F F F
 0.3332979416165465 0.8334492952786110 0.1376953514639299 T T T
 0.0555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.2222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.4996052898163335 0.8342284875011935 0.1383380925362138 T T T
 0.7222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.5555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.9444400000000002 0.8888900000000035 0.0678399999999968 F F F
 0.6672446587077232 0.8350529239810872 0.1379961806186045 T T T
 0.6111099999999965 0.8888900000000035 0.0678399999999968 F F F
 0.7222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.8346777280444277 0.8350826026243828 0.1380389977352261 T T T
 0.4444400000000002 0.8888900000000035 0.0678399999999968 F F F
 0.3888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.7777799999999999 0.8888900000000035 0.0678399999999968 F F F
 0.4855134087457345 0.5243917111685823 0.1940060871978535 T T T
 0.4842142755266121 0.3878977973108229 0.3077054046892321 T T T
 0.6774087493690353 0.4910077553644725 0.1966259293559076 T T T
 0.4755259922078658 0.4273153269076878 0.2523857542085244 T T T
 0.4960166283594869 0.3373014861542976 0.3212846366964140 T T T
 0.4163259434726550 0.3727805948465697 0.3150530725832218 T T T
 0.5313200623493939 0.4532020752071143 0.3208936310687067 T T T
 0.5565268768057077 0.4032672498081598 0.2576443435878715 T T T
 0.4757386427313418 0.5401398440377383 0.2260008497821210 T T T
 0.4934579184998683 0.3865885084155412 0.2662887433792812 T T T
 0.6819995022342129 0.4826539062340411 0.2299651058515611 T T T

Optimized structure of methylamine interacting with three cyanides adsorbed on the Au surface

1.000000000000000
 8.651400000000006 -14.9846643566009998 0.0000000000000000
 8.651400000000006 14.9846643566009998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 34.7092000000000027

Au C H N

108 4 5 4

Selective dynamics

Direct

-0.0000162924462226 0.0010446706624595 0.1381232384697931 T T T
0.1111099999999965 0.0555599999999998 0.0678399999999968 F F F
0.5555599999999998 0.6111099999999965 0.0000000000000000 F F F
0.0555599999999998 0.1111099999999965 0.0000000000000000 F F F
0.1654399692885982 0.9991482051596343 0.1384530781666897 T T T
0.2777799999999999 0.0555599999999998 0.0678399999999968 F F F
0.2222200000000001 0.1111099999999965 0.0000000000000000 F F F
0.3328371296514536 0.9992162335624873 0.1379827164901567 T T T
0.4444400000000002 0.0555599999999998 0.0678399999999968 F F F
0.3888900000000035 0.1111099999999965 0.0000000000000000 F F F
0.4999916096292516 0.9990487274418012 0.1381482991990266 T T T
0.6111099999999965 0.0555599999999998 0.0678399999999968 F F F
0.5555599999999998 0.1111099999999965 0.0000000000000000 F F F
0.7777799999999999 0.0555599999999998 0.0678399999999968 F F F
0.4444400000000002 0.2222200000000001 0.0678399999999968 F F F
0.7222200000000001 0.1111099999999965 0.0000000000000000 F F F
0.8888900000000035 0.4444400000000002 0.0000000000000000 F F F
0.9444400000000002 0.0555599999999998 0.0678399999999968 F F F
0.8888900000000035 0.1111099999999965 0.0000000000000000 F F F
0.9992066276370617 0.1669346536729931 0.1377758694912758 T T T
0.0555599999999998 0.2777799999999999 0.0000000000000000 F F F
0.1641337386620133 0.1656109096142016 0.1382214536191314 T T T
0.2222200000000001 0.2777799999999999 0.0000000000000000 F F F
0.3277858750055893 0.1626148041825156 0.1367127581547707 T T T
0.6672073827367992 0.0006192674342593 0.1379766109661932 T T T
0.1111099999999965 0.2222200000000001 0.0678399999999968 F F F
0.8339435085760325 0.0014364213437587 0.1380929796691609 T T T
0.6111099999999965 0.2222200000000001 0.0678399999999968 F F F
0.7222200000000001 0.2777799999999999 0.0000000000000000 F F F
0.7777799999999999 0.2222200000000001 0.0678399999999968 F F F
0.8336260235862365 0.1665923732059440 0.1381532573398347 T T T
0.9444400000000002 0.2222200000000001 0.0678399999999968 F F F
0.1111099999999965 0.3888900000000035 0.0678399999999968 F F F
0.9995947541501717 0.3333613645294606 0.1379078345937240 T T T
0.2777799999999999 0.3888900000000035 0.0678399999999968 F F F
0.0555599999999998 0.4444400000000002 0.0000000000000000 F F F
0.8888900000000035 0.2777799999999999 0.0000000000000000 F F F

0.5555599999999998 0.2777799999999999 0.0000000000000000 F F F
 0.6677717589601480 0.1655568102222879 0.1381717739024446 T T T
 0.8352000031782031 0.3326502197285869 0.1383519562404651 T T T
 0.5555599999999998 0.4444400000000002 0.0000000000000000 F F F
 0.1637354945974138 0.3328538095502010 0.1382220103288725 T T T
 0.2222200000000001 0.4444400000000002 0.0000000000000000 F F F
 0.3272309890733315 0.3315377398598302 0.1366795197598559 T T T
 0.4444400000000002 0.3888900000000035 0.067839999999968 F F F
 0.3888900000000035 0.4444400000000002 0.0000000000000000 F F F
 0.4966214633598835 0.3318535449285197 0.1371587306191343 T T T
 0.3888900000000035 0.2777799999999999 0.0000000000000000 F F F
 0.6711499789057139 0.3318769217134304 0.1363804870759570 T T T
 0.7777799999999999 0.3888900000000035 0.067839999999968 F F F
 0.7222200000000001 0.4444400000000002 0.0000000000000000 F F F
 0.5009207477222081 0.1627962596881356 0.1372820641454904 T T T
 0.9444400000000002 0.3888900000000035 0.067839999999968 F F F
 0.0019141671289383 0.8351500451855998 0.1380505612013269 T T T
 0.2777799999999999 0.2222200000000001 0.067839999999968 F F F
 0.1111099999999965 0.5555599999999998 0.067839999999968 F F F
 0.3888900000000035 0.7777799999999999 0.0000000000000000 F F F
 0.6111099999999965 0.3888900000000035 0.067839999999968 F F F
 0.1655854230307640 0.5007908919267270 0.1382010561027352 T T T
 0.2777799999999999 0.5555599999999998 0.067839999999968 F F F
 0.2222200000000001 0.6111099999999965 0.0000000000000000 F F F
 0.3280898274825544 0.4997598937990292 0.1370182976888054 T T T
 0.4444400000000002 0.5555599999999998 0.067839999999968 F F F
 0.3888900000000035 0.6111099999999965 0.0000000000000000 F F F
 0.6111099999999965 0.5555599999999998 0.067839999999968 F F F
 0.6733428205069919 0.5039533483592655 0.1376966707544450 T T T
 0.7777799999999999 0.5555599999999998 0.067839999999968 F F F
 0.5011707667274035 0.6725283903375565 0.1368152337950560 T T T
 0.7222200000000001 0.6111099999999965 0.0000000000000000 F F F
 0.9444400000000002 0.5555599999999998 0.067839999999968 F F F
 0.8888900000000035 0.6111099999999965 0.0000000000000000 F F F
 0.0017850934476971 0.6678081123610702 0.1381017258588490 T T T
 0.1111099999999965 0.7222200000000001 0.067839999999968 F F F
 0.0555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.1670903480494465 0.6673950316532159 0.1380698801988227 T T T

0.2777799999999999 0.7222200000000001 0.067839999999968 F F F
 0.2222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.3328528484767618 0.6677727541998321 0.1380430945967714 T T T
 0.4444400000000002 0.7222200000000001 0.067839999999968 F F F
 0.0018574388890446 0.5008015967078024 0.1381883841882150 T T T
 0.8385972120750950 0.5001678149751239 0.1371844817388956 T T T
 0.4993143392287301 0.5041955495386494 0.1372855817442458 T T T
 0.0555599999999998 0.6111099999999965 0.0000000000000000 F F F
 0.8888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.6712068000793204 0.6735794216739864 0.1366623673288432 T T T
 0.7777799999999999 0.7222200000000001 0.067839999999968 F F F
 0.6111099999999965 0.7222200000000001 0.067839999999968 F F F
 0.8384850411236686 0.6722052358202919 0.1371265996400138 T T T
 0.9444400000000002 0.7222200000000001 0.067839999999968 F F F
 0.8888900000000035 0.7777799999999999 0.0000000000000000 F F F
 0.1111099999999965 0.8888900000000035 0.067839999999968 F F F
 0.5555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.1671947533297173 0.8337045552172870 0.1380252535589848 T T T
 0.2777799999999999 0.8888900000000035 0.067839999999968 F F F
 0.3330944272423133 0.8336310034546714 0.1380892309213655 T T T
 0.0555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.2222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.4998802301266420 0.8350301492538590 0.1380718420811606 T T T
 0.7222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.5555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.9444400000000002 0.8888900000000035 0.067839999999968 F F F
 0.6681783500218103 0.8364464916554456 0.1380930280310772 T T T
 0.6111099999999965 0.8888900000000035 0.067839999999968 F F F
 0.7222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.8356908586573597 0.8368024277093857 0.1384536119772682 T T T
 0.4444400000000002 0.8888900000000035 0.067839999999968 F F F
 0.3888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.7777799999999999 0.8888900000000035 0.067839999999968 F F F
 0.4791738537979995 0.5210322049949521 0.1935712646840813 T T T
 0.4884407183596841 0.3947928436704261 0.3134147640697015 T T T
 0.4883039037267534 0.2766484901615150 0.1901577436982065 T T T
 0.6796248642779492 0.4980485124098021 0.1958457322978325 T T T
 0.4885736841489132 0.4571924378090969 0.2611951293842611 T T T

0.4956043870871331 0.3369850633963413 0.3210994881761038 T T T
 0.4195978188653722 0.3784684980281204 0.3194399611860168 T T T
 0.5326707165932855 0.4502533867578012 0.3330331726599358 T T T
 0.5684893226627049 0.4272151978521811 0.2633019024613305 T T T
 0.4627009614388521 0.5333467869714237 0.2250371668369421 T T T
 0.5085273589341165 0.4164027466990955 0.2735494753264667 T T T
 0.4825933383779594 0.2375719604448590 0.2187946438905671 T T T
 0.6850261184993078 0.4925925016231721 0.2293162636902295 T T T

Optimized structure of acetonitrile adsorbed on the on-top site for the 6 × 6 Au (111) surface

1.000000000000000
 8.6514000000000006 -14.9846643566009998 0.000000000000000
 8.6514000000000006 14.9846643566009998 0.000000000000000
 0.000000000000000 0.000000000000000 34.7092000000000027

Au C H N

108 2 3 1

Selective dynamics

Direct

0.0001014281364340 0.0000210207726084 0.1373398660525269 T T T
 0.3888900000000035 0.7777799999999999 0.000000000000000 F F F
 0.0000450257109545 0.5000418096800983 0.1373104157344417 T T T
 0.4444400000000002 0.7222000000000001 0.067839999999968 F F F
 0.3332830981276932 0.6668868906199582 0.1374737489998557 T T T
 0.2222200000000001 0.7777799999999999 0.000000000000000 F F F
 0.2777799999999999 0.7222000000000001 0.067839999999968 F F F
 0.1667110503936747 0.6667822556145772 0.1373765514538086 T T T
 0.0555599999999998 0.7777799999999999 0.000000000000000 F F F
 0.1111099999999965 0.7222000000000001 0.067839999999968 F F F
 0.0000507564010728 0.6667076049843434 0.1373361092527085 T T T
 0.8888900000000035 0.6111099999999965 0.000000000000000 F F F
 0.9444400000000002 0.5555599999999998 0.067839999999968 F F F
 0.8338587261395224 0.4999286653972621 0.1375255483327323 T T T
 0.7222200000000001 0.6111099999999965 0.000000000000000 F F F
 0.7777799999999999 0.5555599999999998 0.067839999999968 F F F
 0.6681904552946457 0.4997761643256838 0.1368503452349649 T T T
 0.6111099999999965 0.5555599999999998 0.067839999999968 F F F
 0.3888900000000035 0.6111099999999965 0.000000000000000 F F F
 0.4444400000000002 0.5555599999999998 0.067839999999968 F F F

0.3318183268741998 0.4999798030854059 0.1369253999134319 T T T
 0.2222200000000001 0.6111099999999965 0.0000000000000000 F F F
 0.2777799999999999 0.5555599999999998 0.0678399999999968 F F F
 0.1660895859277569 0.4999144609114645 0.1375288134891801 T T T
 0.5004107163084779 0.6684551715087420 0.1368183481242711 T T T
 0.5002341907946075 0.5003490330739605 0.1365820938878148 T T T
 0.7222200000000001 0.7777799999999999 0.0000000000000000 F F F
 0.7777799999999999 0.7222000000000001 0.0678399999999968 F F F
 0.1111099999999965 0.5555599999999998 0.0678399999999968 F F F
 0.6682484594880336 0.6684852712382696 0.1368084903897456 T T T
 0.8888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.5000796465797878 0.8338681297411957 0.1375477507643654 T T T
 0.6111099999999965 0.8888900000000035 0.0678399999999968 F F F
 0.5555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.9444400000000002 0.8888900000000035 0.0678399999999968 F F F
 0.6670575049055508 0.8339888705126151 0.1374410250682470 T T T
 0.7777799999999999 0.8888900000000035 0.0678399999999968 F F F
 0.7222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.8340896384915993 0.8340309630101972 0.1376716667498042 T T T
 0.6111099999999965 0.3888900000000035 0.0678399999999968 F F F
 0.4444400000000002 0.8888900000000035 0.0678399999999968 F F F
 0.2222200000000001 0.9444400000000002 0.0000000000000000 F F F
 0.5555599999999998 0.7777799999999999 0.0000000000000000 F F F
 0.3332281707306650 0.8333403940242451 0.1373719191686143 T T T
 0.2777799999999999 0.8888900000000035 0.0678399999999968 F F F
 0.1666869094498499 0.8333361271501206 0.1373238693443848 T T T
 0.0555599999999998 0.9444400000000002 0.0000000000000000 F F F
 0.1111099999999965 0.8888900000000035 0.0678399999999968 F F F
 0.8888900000000035 0.7777799999999999 0.0000000000000000 F F F
 0.9444400000000002 0.7222200000000001 0.0678399999999968 F F F
 0.8335931052706547 0.6668686812896479 0.1374360880769447 T T T
 0.6111099999999965 0.7222200000000001 0.0678399999999968 F F F
 0.3888900000000035 0.9444400000000002 0.0000000000000000 F F F
 0.0002226659785276 0.8333467714132824 0.1374038855555663 T T T
 0.0555599999999998 0.6111099999999965 0.0000000000000000 F F F
 0.9444400000000002 0.3888900000000035 0.0678399999999968 F F F
 0.8334857153237553 0.3332082536656009 0.1373824155018742 T T T
 0.2222200000000001 0.2777799999999999 0.0000000000000000 F F F

0.2777799999999999 0.222200000000001 0.067839999999968 F F F
 0.1660977794101668 0.1662108476678779 0.1374979584157774 T T T
 0.0555599999999998 0.2777799999999999 0.0000000000000000 F F F
 0.9998700630994738 0.1666537209649242 0.1373363356502788 T T T
 0.8888900000000035 0.1111099999999965 0.0000000000000000 F F F
 0.9444400000000002 0.0555599999999998 0.067839999999968 F F F
 0.8888900000000035 0.4444400000000002 0.0000000000000000 F F F
 0.7222200000000001 0.1111099999999965 0.0000000000000000 F F F
 0.4444400000000002 0.2222200000000001 0.067839999999968 F F F
 0.1111099999999965 0.2222200000000001 0.067839999999968 F F F
 0.7777799999999999 0.0555599999999998 0.067839999999968 F F F
 0.6111099999999965 0.0555599999999998 0.067839999999968 F F F
 0.4999731488775771 -0.0000737971311674 0.1373126384792924 T T T
 0.3888900000000035 0.1111099999999965 0.0000000000000000 F F F
 0.4444400000000002 0.0555599999999998 0.067839999999968 F F F
 0.3333140643336774 0.9999523654687221 0.1373299984022998 T T T
 0.2222200000000001 0.1111099999999965 0.0000000000000000 F F F
 0.2777799999999999 0.0555599999999998 0.067839999999968 F F F
 0.1667114323345506 -0.0000983002017710 0.1373658858144589 T T T
 0.0555599999999998 0.1111099999999965 0.0000000000000000 F F F
 0.5555599999999998 0.6111099999999965 0.0000000000000000 F F F
 0.1111099999999965 0.0555599999999998 0.067839999999968 F F F
 0.5555599999999998 0.1111099999999965 0.0000000000000000 F F F
 0.8334492938114391 0.0002067012113991 0.1373656354177161 T T T
 0.6667761361545536 0.0001839174353647 0.1373673517189590 T T T
 0.7222200000000001 0.2777799999999999 0.0000000000000000 F F F
 0.5000664740477647 0.1660519308173142 0.1375488353880992 T T T
 0.7222200000000001 0.4444400000000002 0.0000000000000000 F F F
 0.7777799999999999 0.3888900000000035 0.067839999999968 F F F
 0.6670508421498959 0.3329644986005418 0.1374679999592068 T T T
 0.3888900000000035 0.2777799999999999 0.0000000000000000 F F F
 0.5003816601776426 0.3319972004431004 0.1369010661055135 T T T
 0.3888900000000035 0.4444400000000002 0.0000000000000000 F F F
 0.4444400000000002 0.3888900000000035 0.067839999999968 F F F
 0.6111099999999965 0.2222200000000001 0.067839999999968 F F F
 0.2222200000000001 0.4444400000000002 0.0000000000000000 F F F
 0.1662465077531196 0.3331874483480139 0.1375349203553018 T T T
 0.3319284002114133 0.3319381401887846 0.1369237135550776 T T T

0.3332237655874926 0.1663829414813479 0.1374735676763053 T T T
 0.7777799999999999 0.2222000000000001 0.0678399999999968 F F F
 0.8333510239139073 0.1666554478145833 0.1376645480942040 T T T
 0.5555599999999998 0.4444400000000002 0.0000000000000000 F F F
 0.1111099999999965 0.3888900000000035 0.0678399999999968 F F F
 0.9998590418156117 0.3332177592528950 0.1373366512140050 T T T
 0.9444400000000002 0.2222000000000001 0.0678399999999968 F F F
 0.0555599999999998 0.4444400000000002 0.0000000000000000 F F F
 0.8888900000000035 0.2777799999999999 0.0000000000000000 F F F
 0.5555599999999998 0.2777799999999999 0.0000000000000000 F F F
 0.6668026372045395 0.1665384982792485 0.1373733971953894 T T T
 0.2777799999999999 0.3888900000000035 0.0678399999999968 F F F
 0.5052733180105003 0.5054415489838274 0.2387387255234819 T T T
 0.5088101352240593 0.5096775347367746 0.2803350702100263 T T T
 0.5096232119668068 0.4510145799342858 0.2918629810529325 T T T
 0.5692156376266765 0.5702566001275013 0.2898035317404850 T T T
 0.4499104482805645 0.5105902997542979 0.2915429065369660 T T T
 0.5017812843986384 0.5013567850483459 0.2053357354305876 T T T

Optimized structure of Au(CN) complexed with benzene

1.00000000000000
 24.3198560000000015 0.0000000000000000 0.0000000000000000
 0.0000000000000000 25.2223790000000001 0.0000000000000000
 0.0000000000000000 0.0000000000000000 24.9671610000000008

Au C H N

1 7 6 1

Selective dynamics

Direct

0.4847275826393300 0.5006656634324429 0.5471336851994408 T T T
 0.5515130702840381 0.3977953664180447 0.4734192659006524 T T T
 0.5523461332437662 0.4032975999001707 0.5287001098874100 T T T
 0.5027187659035377 0.4124700345404477 0.5571993372500543 T T T
 0.4523185992378629 0.4163934774207050 0.5284743772622775 T T T
 0.4526376937787333 0.4108369760673867 0.4719273445524621 T T T
 0.5016044384910430 0.4015429706062719 0.4450463118543979 T T T
 0.4921723348800384 0.5775872710146785 0.5530503164497063 T T T
 0.5896830517432363 0.3903793967398386 0.4517599537839914 T T T
 0.5908252481137737 0.4001144204038880 0.5508354621286458 T T T

0.5023300227525667 0.4096118277426868 0.6008422341025863 T T T
 0.4132381022205251 0.4167296283603577 0.5500020709788132 T T T
 0.4138815125836999 0.4132596055964157 0.4500794933553678 T T T
 0.5015102795035347 0.3971303308101071 0.4016197964351633 T T T
 0.4970658535433117 0.6236940899845749 0.5569183159840279 T T T

Optimized structure of Au(CN)3 complexed with benzene

1.00000000000000
 24.3198560000000015 0.0000000000000000 0.0000000000000000
 0.0000000000000000 25.2223790000000001 0.0000000000000000
 0.0000000000000000 0.0000000000000000 24.9671610000000008

Au C H N

1 9 6 3

Selective dynamics

Direct

0.4997902536801658 0.5060345480057765 0.5578249266051394 T T T
 0.5501643893962261 0.3948326021301799 0.4699504000305182 T T T
 0.5497828739302704 0.4028452690755415 0.5249522847465153 T T T
 0.4990467082745543 0.4114364052289848 0.5523304186768905 T T T
 0.4488936785824528 0.4065308112868851 0.5231364564759535 T T T
 0.4499414214087569 0.3986692960351233 0.4680569040002041 T T T
 0.5004377142832143 0.3934109823423944 0.4415909151561806 T T T
 0.4173894445703615 0.5093286125637317 0.5608720341191784 T T T
 0.5823095011081902 0.5073465118828653 0.5586624954985847 T T T
 0.5006001314089836 0.5837319217219012 0.5613401774944357 T T T
 0.5010500096432325 0.3876435988551093 0.3982849024556900 T T T
 0.4114701549074609 0.3964086510132967 0.4457914636534815 T T T
 0.5881216618013090 0.4033442137394424 0.5474715841959648 T T T
 0.4981022099056794 0.4082885594598885 0.5960990254061470 T T T
 0.5891110053773384 0.3896659334371838 0.4490205648380788 T T T
 0.4098929682498360 0.4094573797657658 0.5443151805455319 T T T
 0.3693819734122393 0.5109345894603989 0.5635167340781226 T T T
 0.6303984057817980 0.5074318115654736 0.5602081101147867 T T T
 0.5008257114699338 0.6300825687660647 0.5619054968146050 T T T