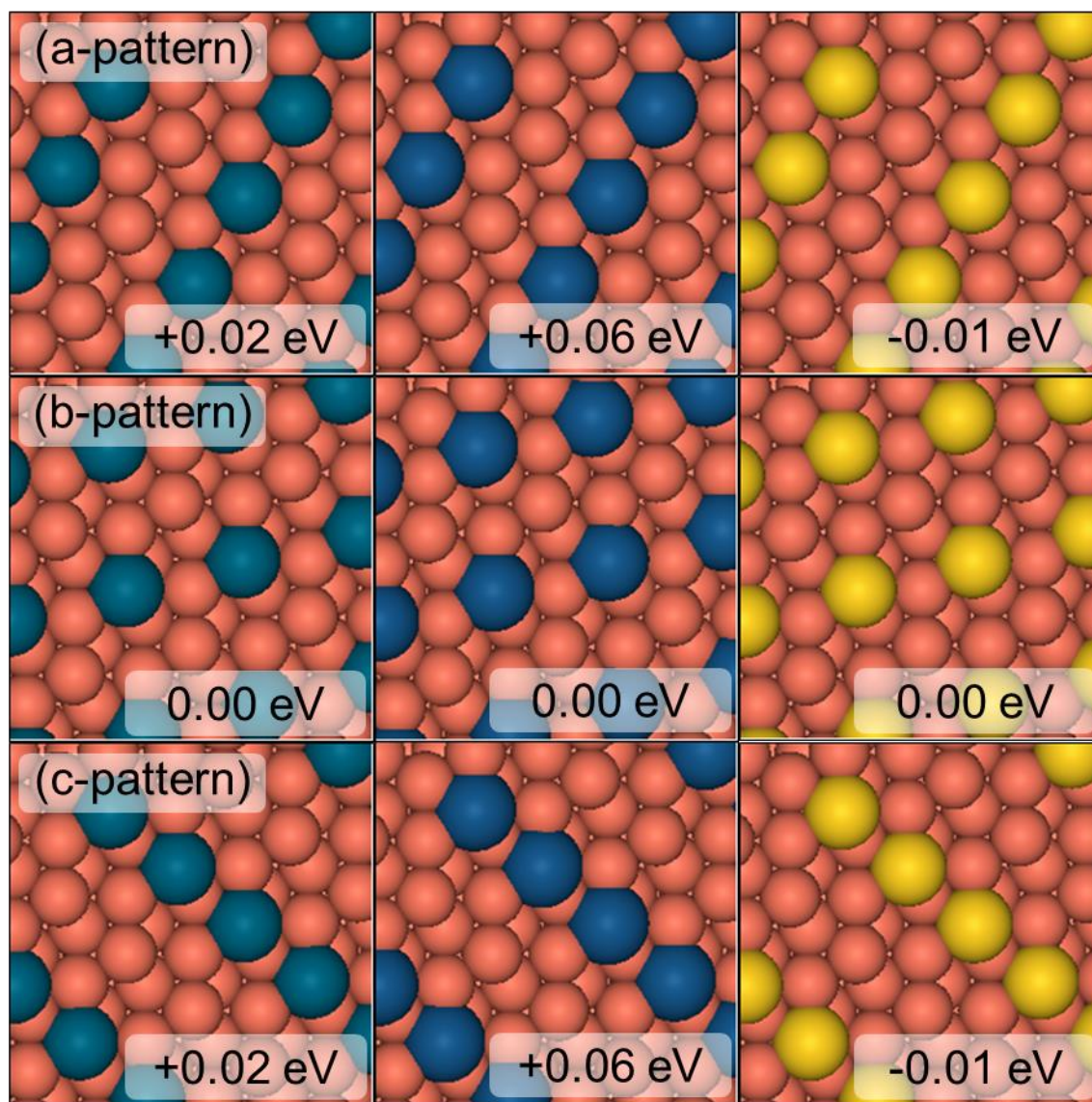


# Tuning the Surface Chemistry of Chiral Cu(531)<sup>S</sup> for Enhanced Enantiospecific Adsorption of Amino Acids

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## Supplementary Information



**Figure S1:** The configurations and energetics relative to the b-pattern of 50%-decorated surface structures.

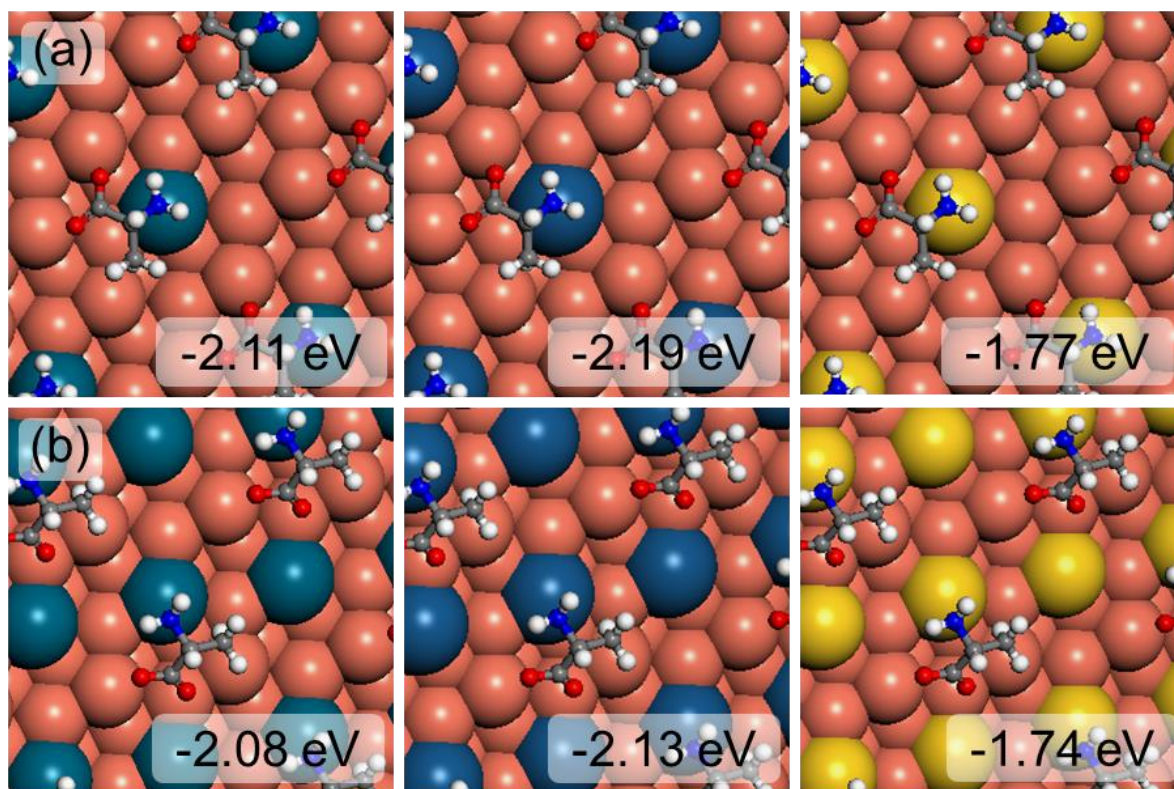
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Figure S1 shows the configurations and energetics relative to b-pattern of 50%-decorated surface structures we examined. Although b-pattern is 0.01 eV less stable than other patterns with Au-decorating, we finally choose b-pattern in 50%-decorated surface because it is 0.02 eV and 0.06 eV more stable than other patterns with Pd- and Pt-decorating, respectively.

|                                                                                |          | $E_{\text{ads}}$ | $\text{Diff}_{\text{ads}}$ | $ \Delta E_{\text{enan}} $ | $\text{Diff}_{\text{enan}}$ |
|--------------------------------------------------------------------------------|----------|------------------|----------------------------|----------------------------|-----------------------------|
| <b><math>\mu_4</math>-serine<br/>on pure Cu(531)<sup>S</sup></b>               | <b>D</b> | -2.26            | 0.03                       | 0.13                       | 0.01                        |
|                                                                                | <b>L</b> | -2.13            | 0.04                       |                            |                             |
| <b><math>\mu_4</math>-serine<br/>on Au-25%-decorated Cu(531)<sup>S</sup></b>   | <b>D</b> | -1.98            | 0.08                       | 0.13                       | 0.01                        |
|                                                                                | <b>L</b> | -1.85            | 0.09                       |                            |                             |
| <b><math>\mu_4</math>-cysteine<br/>on pure Cu(531)<sup>S</sup></b>             | <b>D</b> | -3.25            | 0.06                       | 0.10                       | 0.01                        |
|                                                                                | <b>L</b> | -3.35            | 0.04                       |                            |                             |
| <b><math>\mu_4</math>-cysteine<br/>on Au-50%-decorated Cu(531)<sup>S</sup></b> | <b>D</b> | -2.63            | 0.07                       | 0.18                       | 0.01                        |
|                                                                                | <b>L</b> | -2.81            | 0.06                       |                            |                             |

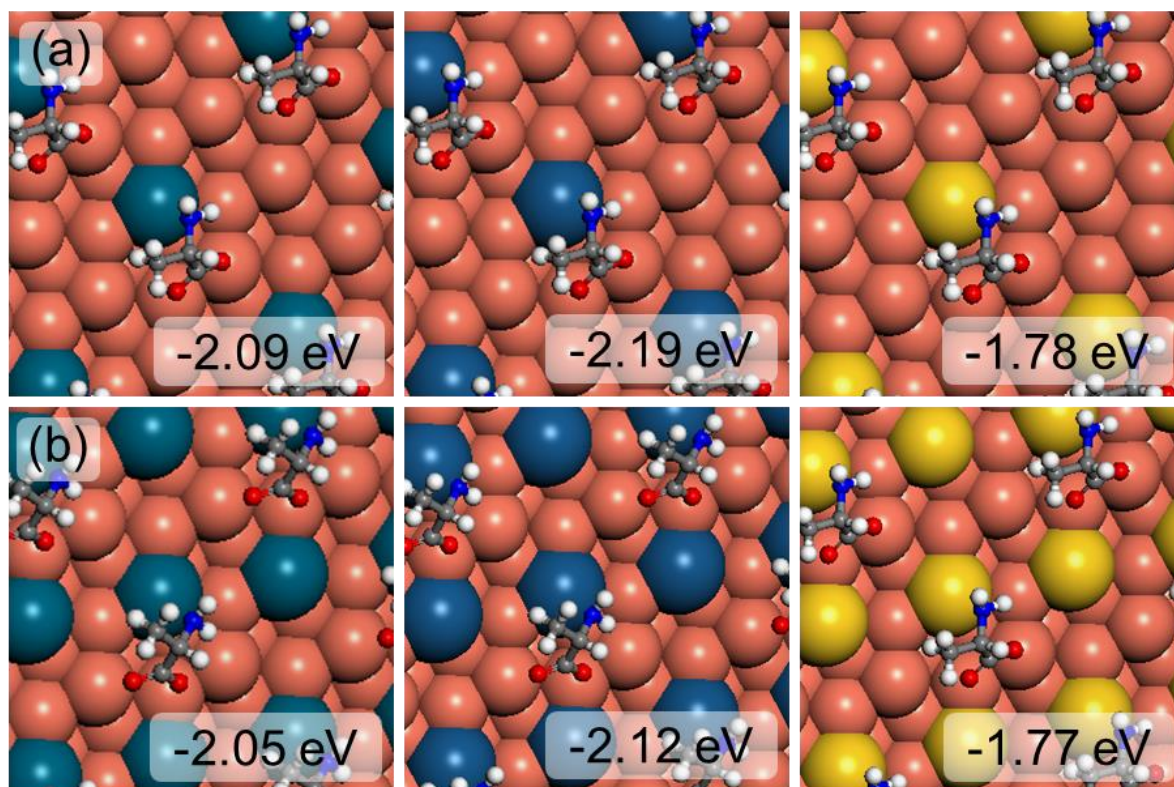
**Table S1:**  $E_{\text{ads}}$  and  $|\Delta E_{\text{enan}}|$  of  $\mu_4$ -serine and  $\mu_4$ -cysteine on pure and decorated Cu(531)<sup>S</sup> for concentration dependence.  $E_{\text{ads}}$  is the adsorption energy of amino acids on these surfaces.  $\text{Diff}_{\text{ads}}$  and  $\text{Diff}_{\text{enan}}$  are energy difference from  $E_{\text{ads}}$  and  $|\Delta E_{\text{enan}}|$  of our original calculations, respectively.

We performed the test calculations for the adsorption of both enantiomers of  $\mu_4$ -serine and  $\mu_4$ -cysteine with four times lower coverage. There were slight interactions between the adsorbates on the coverage we originally used. However, the enantiospecific adsorption energy differences do not have significant changes between the two coverages, which does not change our key results in this paper.



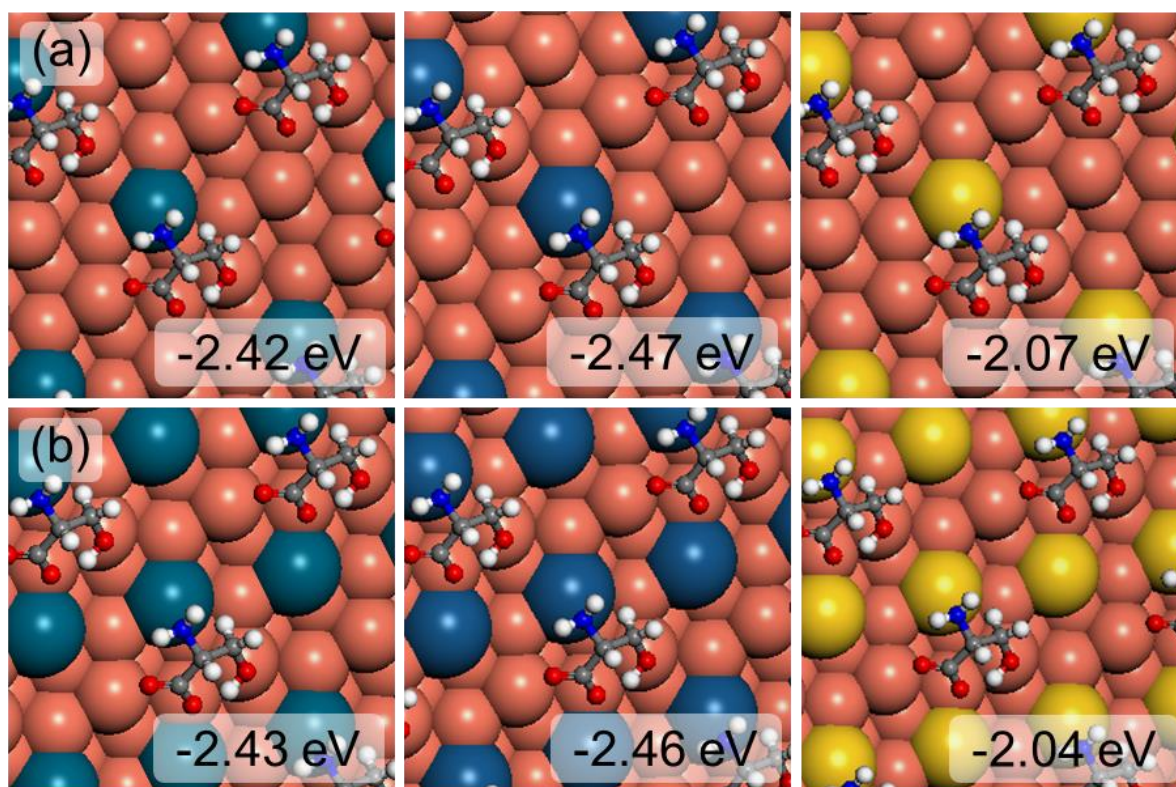
**Figure S2:** Top views of the most favorable adsorption configuration and energetic of D-alanine on (a) Pd-, Pt-, and Au-25%-decorated (b) Pd-, Pt-, and Au-50%-decorated Cu(531)<sup>S</sup>, respectively.

Figure S2 shows the most favorable adsorption configuration and energetic of D-alanine on Pd-, Pt-, and Au-decorated surfaces. The most stable D-alanine has the adsorption energy of -2.19 eV on Pt-25%-decorated surfaces, while the most unstable D-alanine has the adsorption energy of -1.74 eV on Au-50%-decorated surfaces. For all cases, the more kink sites is decorated, the weaker the adsorption energy is.



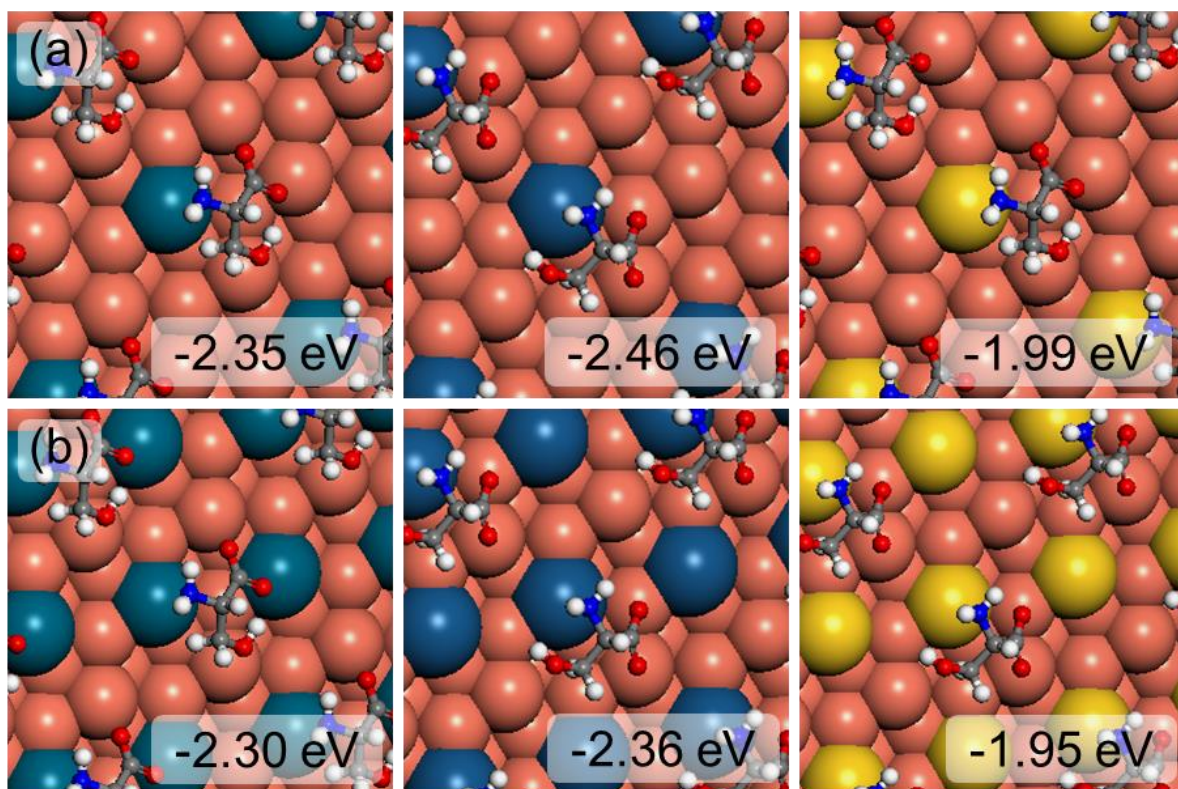
**Figure S3:** Top views of the most favorable adsorption configuration and energetic of L-alanine on (a) Pd-, Pt-, and Au-25%-decorated (b) Pd-, Pt-, and Au-50%-decorated Cu(531)<sup>S</sup>, respectively.

Figure S3 shows the most favorable adsorption configuration and energetic of L-alanine on Pd-, Pt-, and Au-decorated surfaces. The most stable L-alanine has the adsorption energy of -2.19 eV on Pt-25%-decorated surfaces, while the most unstable L-alanine has the adsorption energy of -1.77 eV on Au-50%-decorated surfaces. For all cases, the more kink sites is decorated, the weaker the adsorption energy is.



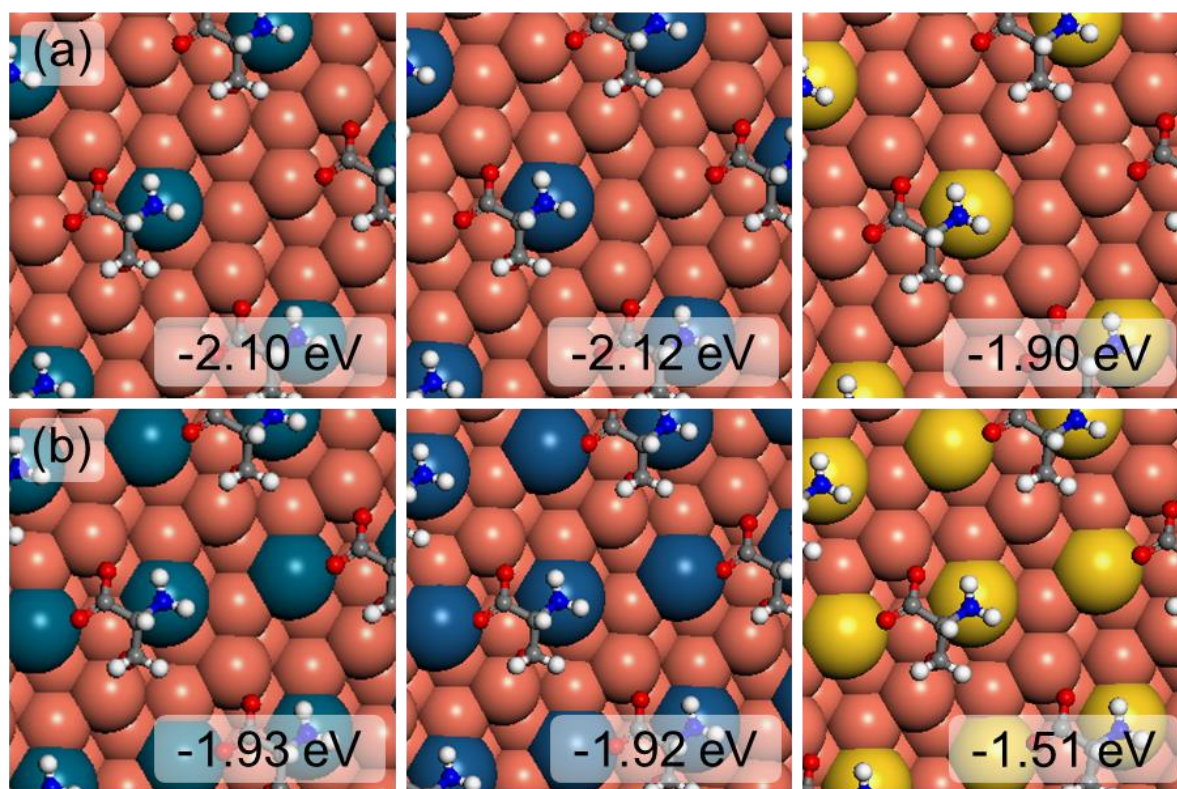
**Figure S4:** Top views of the most favorable adsorption configuration and energetic of D-μ<sub>3</sub>-serine on (a) Pd-, Pt-, and Au-25%-decorated (b) Pd-, Pt-, and Au-50%-decorated Cu(531)<sup>S</sup>, respectively.

Figure S4 shows the most favorable adsorption configuration and energetic of D-μ<sub>3</sub>-serine on Pd-, Pt-, and Au-decorated surfaces. The most stable D-μ<sub>3</sub>-serine has the adsorption energy of -2.47 eV on Pt-25%-decorated surfaces, while the most unstable D-μ<sub>3</sub>-serine has the adsorption energy of -2.04 eV on Au-50%-decorated surfaces. For all cases, the more kink sites is decorated, the weaker the adsorption energy is.



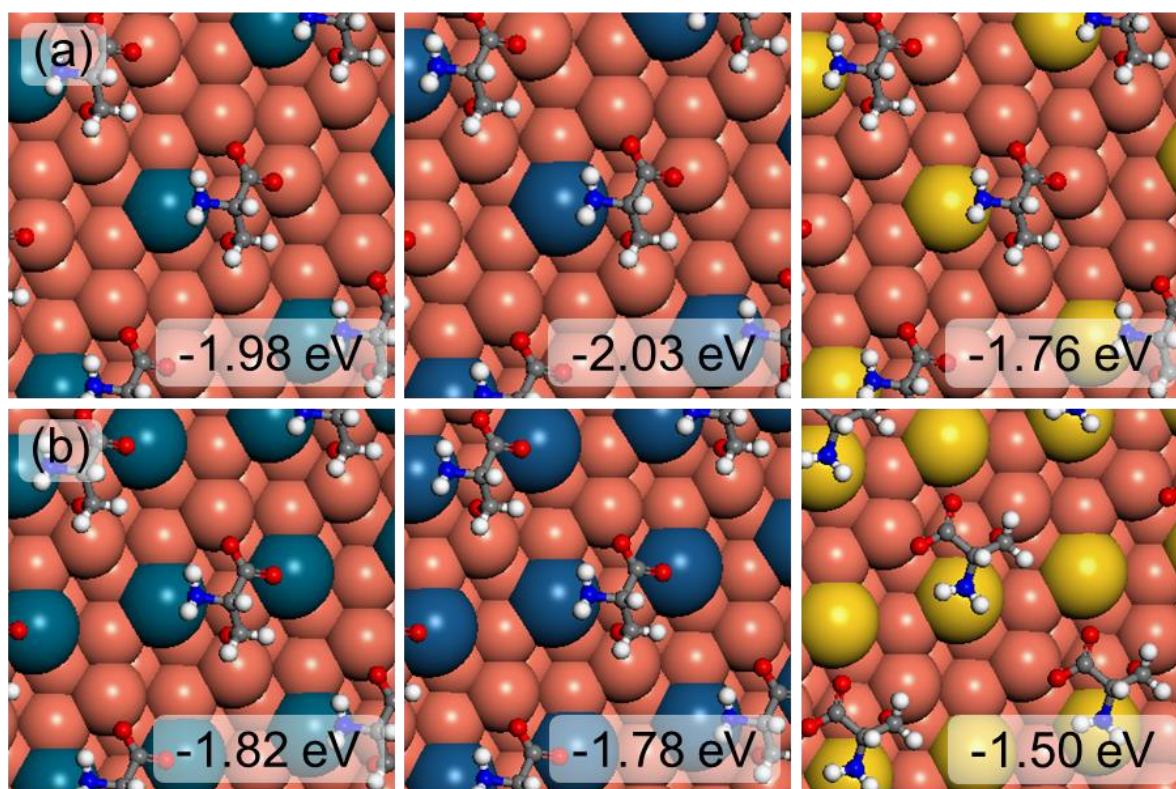
**Figure S5:** Top views of the most favorable adsorption configuration and energetic of L-μ<sub>3</sub>-serine on (a) Pd-, Pt-, and Au-25%-decorated (b) Pd-, Pt-, and Au-50%-decorated Cu(531)<sup>S</sup>, respectively.

Figure S5 shows the most favorable adsorption configuration and energetic of L-μ<sub>3</sub>-serine on Pd-, Pt-, and Au-decorated surfaces. The most stable L-μ<sub>3</sub>-serine has the adsorption energy of -2.46 eV on Pt-25%-decorated surfaces, while the most unstable L-μ<sub>3</sub>-serine has the adsorption energy of -1.95 eV on Au-50%-decorated surfaces. For all cases, the more kink sites is decorated, the weaker the adsorption energy is.



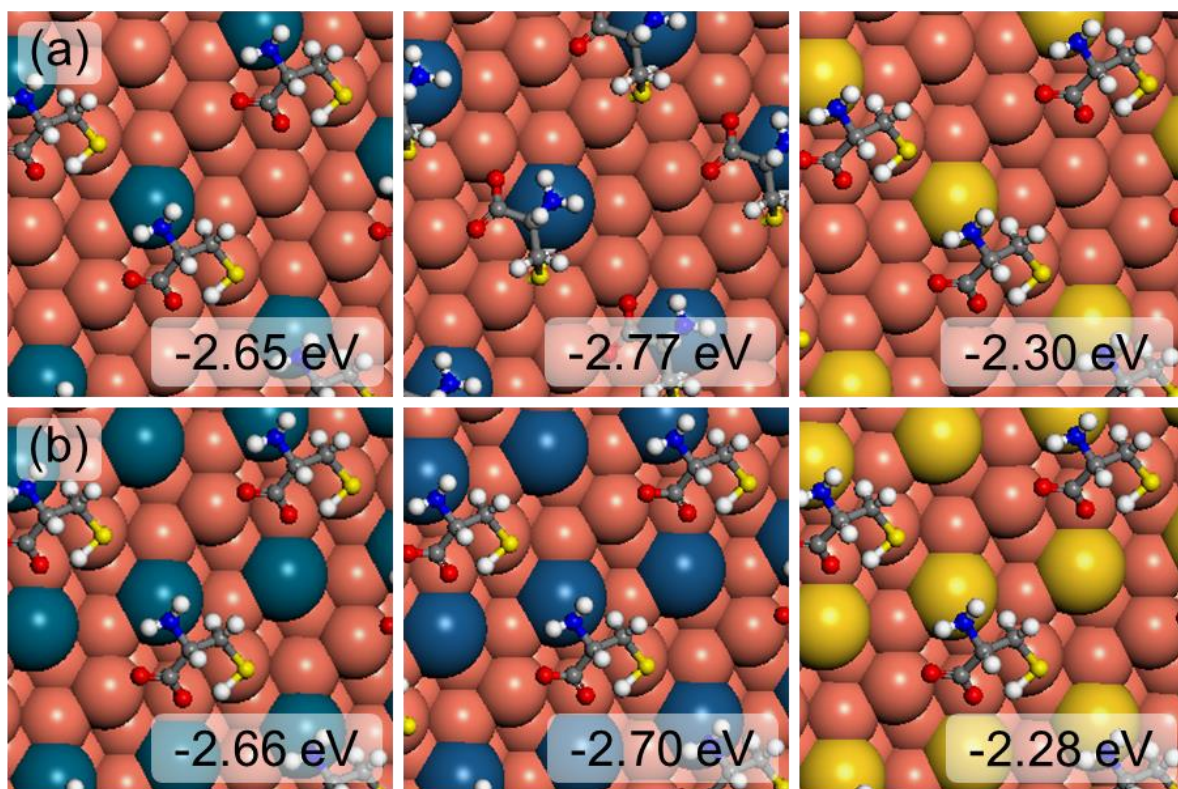
**Figure S6:** Top views of the most favorable adsorption configuration and energetic of D- $\mu_4$ -serine on (a) Pd-, Pt-, and Au-25%-decorated (b) Pd-, Pt-, and Au-50%-decorated Cu(531)<sup>S</sup>, respectively.

Figure S6 shows the most favorable adsorption configuration and energetic of D- $\mu_4$ -serine on Pd-, Pt-, and Au-decorated surfaces. The most stable D- $\mu_4$ -serine has the adsorption energy of -2.23 eV on pure surfaces, while the most unstable D- $\mu_4$ -serine has the adsorption energy of -1.51 eV on Au-50%-decorated surfaces. For all cases, the more kink sites is decorated, the weaker the adsorption energy is.



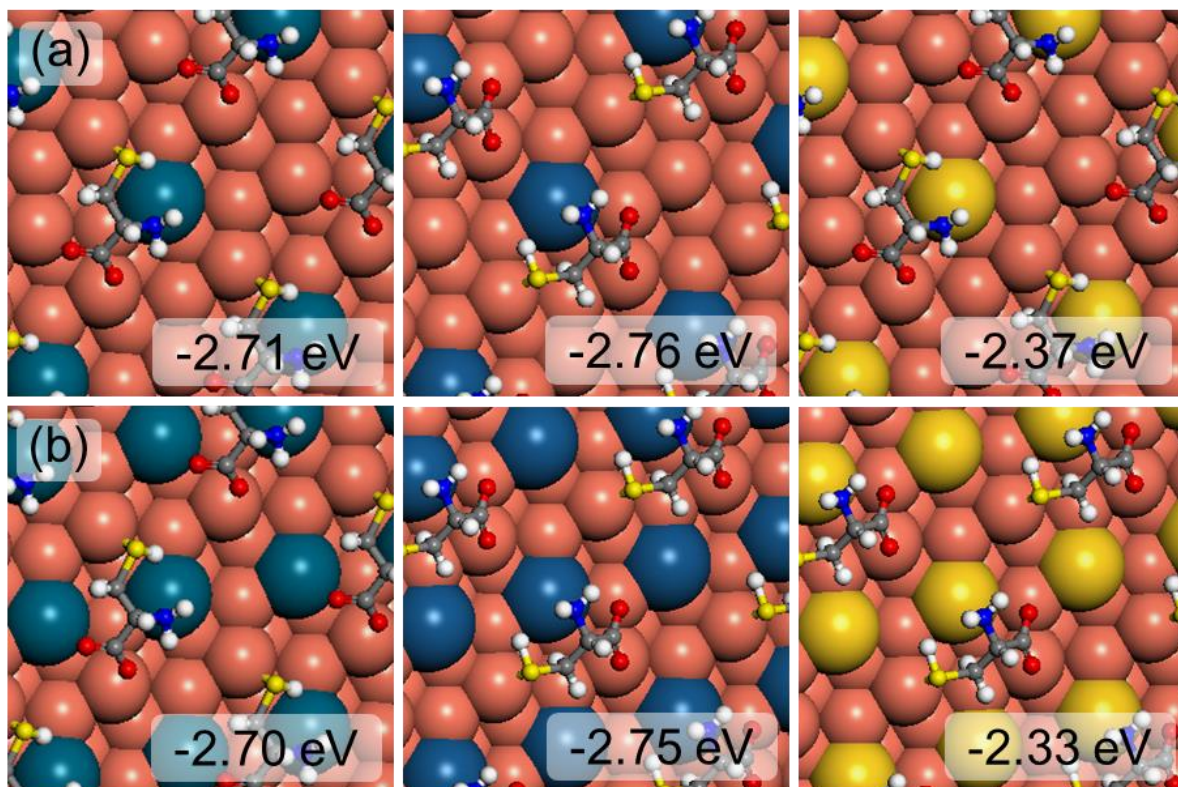
**Figure S7:** Top views of the most favorable adsorption configuration and energetic of L-μ<sub>4</sub>-serine on (a) Pd-, Pt-, and Au-25%-decorated (b) Pd-, Pt-, and Au-50%-decorated Cu(531)<sup>S</sup>, respectively.

Figure S7 shows the most favorable adsorption configuration and energetic of L-μ<sub>4</sub>-serine on Pd-, Pt-, and Au-decorated surfaces. The most stable L-μ<sub>4</sub>-serine has the adsorption energy of -2.09 eV on pure surfaces, while the most unstable L-μ<sub>4</sub>-serine has the adsorption energy of -1.50 eV on Au-50%-decorated surfaces. For all cases, the more kink sites is decorated, the weaker the adsorption energy is.



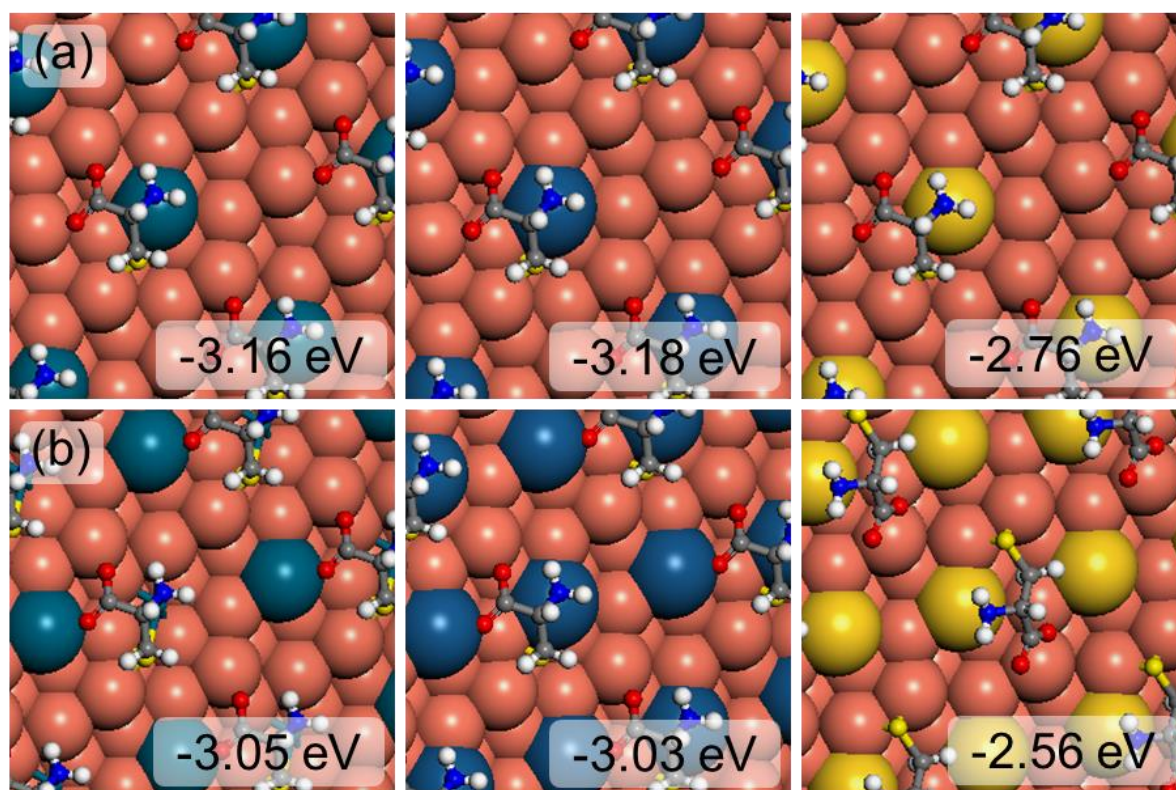
**Figure S8:** Top views of the most favorable adsorption configuration and energetic of D- $\mu_3$ -cysteine on (a) Pd-, Pt-, and Au-25%-decorated (b) Pd-, Pt-, and Au-50%-decorated Cu(531)<sup>S</sup>, respectively.

Figure S8 shows the most favorable adsorption configuration and energetic of D- $\mu_3$ -cysteine on Pd-, Pt-, and Au-decorated surfaces. The most stable D- $\mu_3$ -cysteine has the adsorption energy of -2.77 eV on Pt-25%-decorated surfaces, while the most unstable D- $\mu_3$ -cysteine has the adsorption energy of -2.28 eV on Au-50%-decorated surfaces. For Pt and Au cases, the more kink sites is decorated, the weaker the adsorption energy is. But the adsorption energy of D- $\mu_3$ -cysteine in Pd-25%-decorated Cu(531)<sup>S</sup> is 0.01 eV less stable than Pd-50%-decorated Cu(531)<sup>S</sup>.



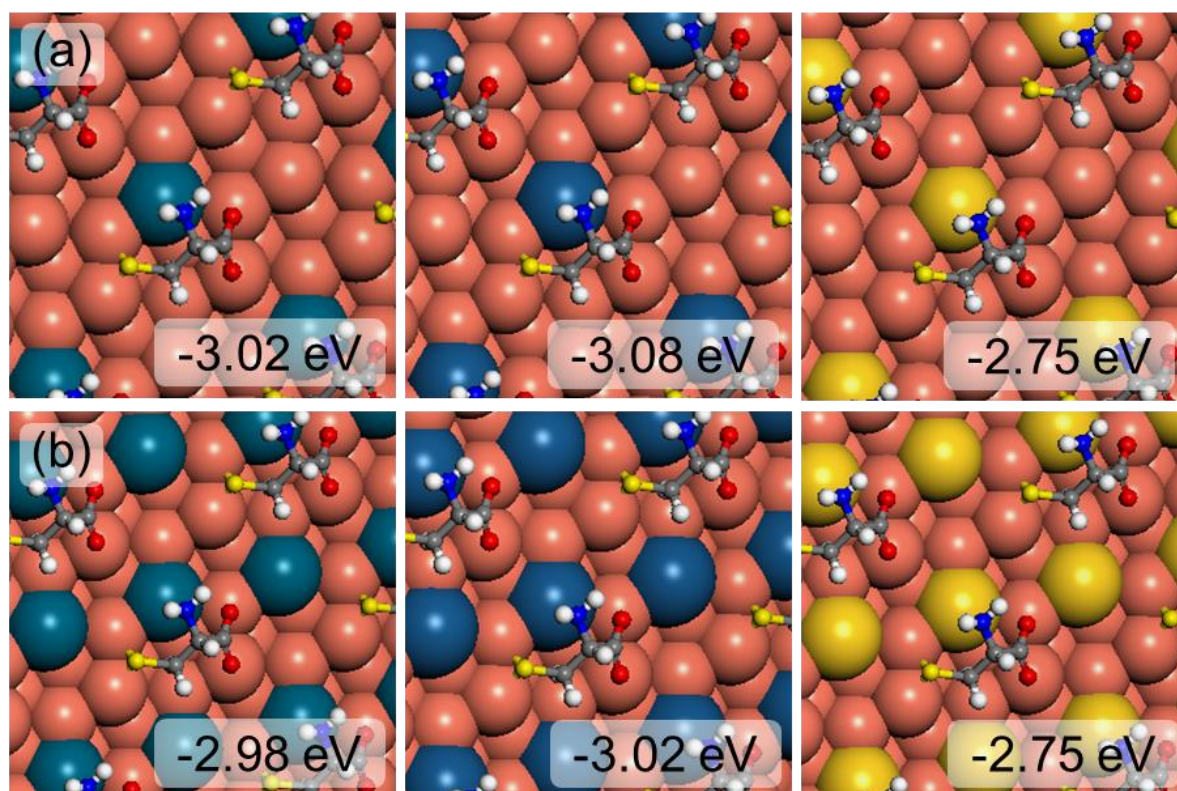
**Figure S9:** Top views of the most favorable adsorption configuration and energetic of L- $\mu_3$ -cysteine on (a) Pd-, Pt-, and Au-25%-decorated (b) Pd-, Pt-, and Au-50%-decorated Cu(531)<sup>S</sup>, respectively.

Figure S9 shows the most favorable adsorption configuration and energetic of L- $\mu_3$ -cysteine on Pd-, Pt-, and Au-decorated surfaces. The most stable L- $\mu_3$ -cysteine has the adsorption energy of -2.76 eV on Pt-25%-decorated surfaces, while the most unstable L- $\mu_3$ -cysteine has the adsorption energy of -2.33 eV on Au-50%-decorated surfaces. For all cases, the more kink sites is decorated, the weaker the adsorption energy is.



**Figure S10:** Top views of the most favorable adsorption configuration and energetic of D- $\mu_4$ -cysteine on (a) Pd-, Pt-, and Au-25%-decorated (b) Pd-, Pt-, and Au-50%-decorated Cu(531)<sup>S</sup>, respectively.

Figure S10 shows the most favorable adsorption configuration and energetic of D- $\mu_4$ -cysteine on Pd-, Pt-, and Au-decorated surfaces. The most stable D- $\mu_4$ -cysteine has the adsorption energy of -3.19 eV on pure surfaces, while the most unstable D- $\mu_4$ -cysteine has the adsorption energy of -2.56 eV on Au-50%-decorated surfaces. For all cases, the more kink sites is decorated, the weaker the adsorption energy is.

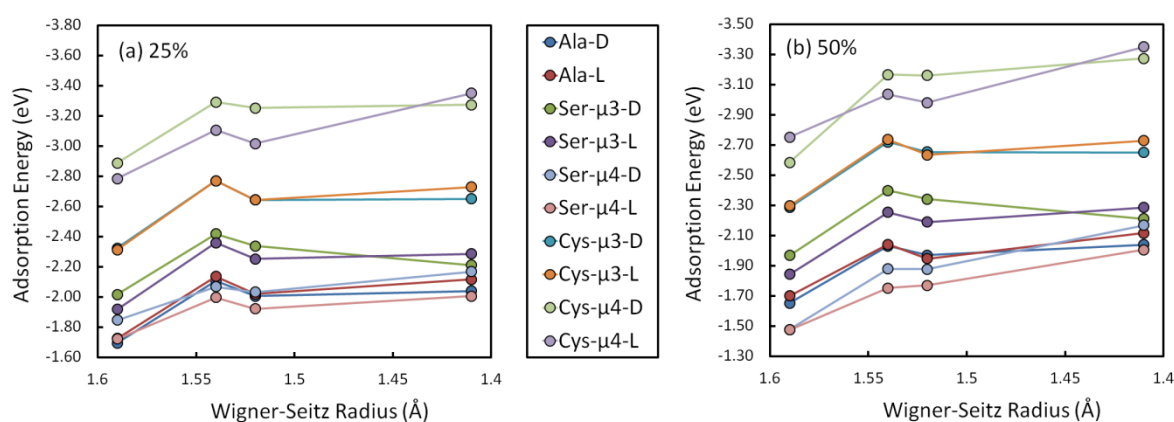


**Figure S11:** Top views of the most favorable adsorption configuration and energetic of L- $\mu_4$ -cysteine on (a) Pd-, Pt-, and Au-25%-decorated (b) Pd-, Pt-, and Au-50%-decorated Cu(531)<sup>S</sup>, respectively.

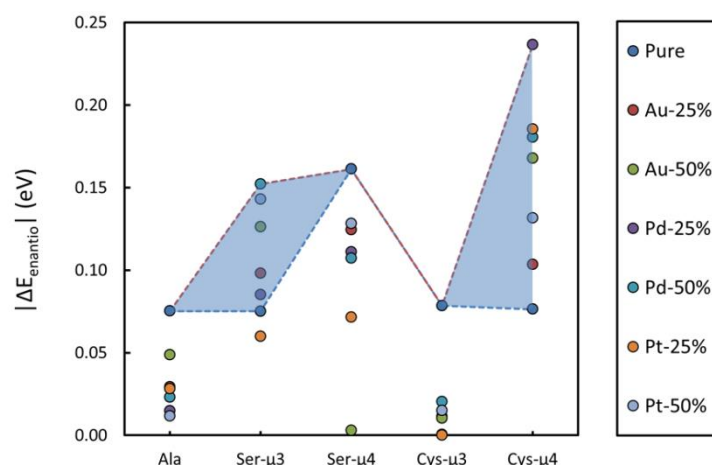
Figure S11 shows the most favorable adsorption configuration and energetic of L- $\mu_4$ -cysteine on Pd-, Pt-, and Au-decorated surfaces. The most stable L- $\mu_4$ -cysteine has the adsorption energy of -3.31 eV on pure surfaces, while the most unstable L- $\mu_4$ -cysteine has the adsorption energy of -2.75 eV on Au-decorated surfaces. For Pd and Pt cases, the more kink sites is decorated, the weaker the adsorption energy is. But the adsorption energy of L- $\mu_4$ -cysteine in Pd-25% and 50%-decorated Cu(531)<sup>S</sup> are very similar to each other.

|                                | Pure  |       | Pd-25% |       | Pt-25% |       | Au-25% |       | Pd-50% |       | Pt-50% |       | Au-50% |       |
|--------------------------------|-------|-------|--------|-------|--------|-------|--------|-------|--------|-------|--------|-------|--------|-------|
|                                | D     | L     | D      | L     | D      | L     | D      | L     | D      | L     | D      | L     | D      | L     |
| <b>Ala</b>                     | -2.04 | -2.12 | -2.01  | -2.02 | -2.11  | -2.14 | -1.70  | -1.72 | -1.97  | -1.95 | -2.03  | -2.04 | -1.65  | -1.70 |
| <b>Ser (<math>\mu</math>3)</b> | -2.21 | -2.29 | -2.34  | -2.25 | -2.42  | -2.36 | -2.02  | -1.92 | -2.34  | -2.19 | -2.40  | -2.25 | -1.97  | -1.84 |
| <b>Ser (<math>\mu</math>4)</b> | -2.17 | -2.01 | -2.03  | -1.92 | -2.07  | -2.00 | -1.85  | -1.72 | -1.88  | -1.77 | -1.88  | -1.75 | -1.48  | -1.48 |
| <b>Cys (<math>\mu</math>3)</b> | -2.65 | -2.73 | -2.64  | -2.64 | -2.77  | -2.77 | -2.32  | -2.31 | -2.65  | -2.63 | -2.72  | -2.74 | -2.29  | -2.30 |
| <b>Cys (<math>\mu</math>4)</b> | -3.27 | -3.35 | -3.25  | -3.02 | -3.29  | -3.11 | -2.89  | -2.78 | -3.16  | -2.98 | -3.17  | -3.04 | -2.59  | -2.75 |

**Table S2:** The adsorption energies (in eV) of both enantiomers of amino acids we examined on each surface by DFT-D3 method.



**Figure S12:** The adsorption energies of amino acids on (a) 25% Pd-, Pt-, and Au-decorated Cu(531)<sup>S</sup> and (b) 50% Pd-, Pt-, and Au-decorated Cu(531)<sup>S</sup> as a function of Wigner-Seitz radius of kink atom by DFT-D3 method.



**Figure S13:**  $|\Delta E_{\text{enantio}}|$  of amino acids on pure and step decorated Cu(531)<sup>S</sup> performed by DFT-D3 method. The blue dashed line indicates  $|\Delta E_{\text{enantio}}|$  of amino acids on pure Cu(531)<sup>S</sup>, and the red dashed line denotes the highest  $|\Delta E_{\text{enantio}}|$  of each amino acid among all surfaces.

To justify the numbers calculated by DFT-D2 method, we also performed DFT-D3 calculations. Although the adsorption energies and the corresponding enantiospecificities are slightly changed, our qualitative result that  $\mu_3$ -serine and  $\mu_4$ -cysteine show the largest enhancement of enantiospecificity upon the step decoration among the amino acids we examined is not changed under the DFT-D3 as can be seen in Fig. S13.

**\* The full set of coordinates for all structures discussed in the text**

Tables S3-S75 list the coordinates for the structures of glycine, alanine, serine and cysteine adsorption we have examined on pure, Pd-, Pt-, and Au-decorated Cu(531)<sup>S</sup>. The coordinates for the adsorbate are defined for a single supercell of a (1×1) surface unit cell with all coordinates in Å . A table defining unit cell vectors for supercell is also listed in Å .

|          | <b>x</b> | <b>y</b> | <b>z</b> |
|----------|----------|----------|----------|
| <b>a</b> | 3.044    | 0.857    | 0.000    |
| <b>b</b> | 1.015    | 2.229    | 0.000    |
| <b>c</b> | 0.000    | 0.000    | 6.994    |

**Table S3:** Unit cell vectors of supercell used for calculations on Cu(531)<sup>S</sup> with a lattice constant of 3.64 Å . (in Å )

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|-------|-------|
| C    | 5.512  | 5.023  | 9.688  | Cu   | 11.032 | 8.052  | 6.257 | Cu   | 8.659  | 5.928 | 3.246 |
| C    | 4.217  | 5.611  | 9.112  | Cu   | 9.178  | 4.055  | 6.265 | Cu   | 6.806  | 1.867 | 3.227 |
| H    | 5.400  | 5.002  | 10.787 | Cu   | 5.485  | 6.526  | 6.126 | Cu   | 3.086  | 4.343 | 3.223 |
| H    | 5.628  | 3.987  | 9.334  | Cu   | 3.605  | 2.453  | 6.218 | Cu   | 1.248  | 0.297 | 3.242 |
| H    | 7.463  | 5.676  | 9.967  | Cu   | 9.074  | 6.526  | 5.696 | Cu   | 2.964  | 6.811 | 2.581 |
| H    | 6.433  | 6.813  | 9.346  | Cu   | 7.244  | 2.495  | 5.618 | Cu   | 1.128  | 2.769 | 2.627 |
| N    | 6.706  | 5.821  | 9.292  | Cu   | 3.554  | 5.005  | 5.572 | Cu   | 8.502  | 8.369 | 2.536 |
| O    | 4.217  | 6.875  | 8.932  | Cu   | 1.671  | 0.910  | 5.651 | Cu   | 6.669  | 4.320 | 2.561 |
| O    | 3.262  | 4.800  | 8.918  | Cu   | -0.284 | -0.646 | 4.984 | Cu   | 12.139 | 8.396 | 1.977 |
|      |        |        |        | Cu   | 1.597  | 3.415  | 5.062 | Cu   | 10.301 | 4.339 | 1.991 |
|      |        |        |        | Cu   | 8.974  | 8.987  | 4.941 | Cu   | 6.591  | 6.818 | 1.957 |
|      |        |        |        | Cu   | 7.143  | 4.964  | 4.998 | Cu   | 4.734  | 2.762 | 1.956 |
| Cu   | 7.429  | 5.566  | 7.367  | Cu   | 12.532 | 9.020  | 4.393 | Cu   | 10.205 | 6.834 | 1.441 |
| Cu   | 5.673  | 1.521  | 7.227  | Cu   | 10.695 | 4.976  | 4.422 | Cu   | 8.352  | 2.782 | 1.428 |
| Cu   | 2.115  | 4.149  | 7.387  | Cu   | 7.010  | 7.460  | 4.366 | Cu   | 4.620  | 5.251 | 1.419 |
| Cu   | 0.121  | -0.119 | 7.343  | Cu   | 5.148  | 3.397  | 4.351 | Cu   | 2.764  | 1.208 | 1.444 |
| Cu   | 12.911 | 9.678  | 6.727  | Cu   | 10.602 | 7.458  | 3.828 | Cu   | 10.104 | 9.330 | 0.949 |
| Cu   | 11.163 | 5.573  | 6.800  | Cu   | 8.755  | 3.416  | 3.809 | Cu   | 8.258  | 5.273 | 0.955 |
| Cu   | 7.421  | 8.095  | 6.719  | Cu   | 5.063  | 5.894  | 3.773 | Cu   | 4.528  | 7.738 | 0.956 |
| Cu   | 5.550  | 3.986  | 6.677  | Cu   | 3.202  | 1.835  | 3.817 | Cu   | 2.666  | 3.688 | 0.942 |

**Table S4:** Coordinates for the most stable glycine adsorbed on pure Cu(531)<sup>S</sup>. This configuration is shown in Fig. 1a.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.457  | 4.757  | 9.969  | Cu   | 10.832 | 8.190  | 6.181 | Cu   | 8.477  | 5.997  | 3.205 |
| C    | 9.776  | 4.623  | 9.211  | Cu   | 9.014  | 4.105  | 6.140 | Cu   | 6.638  | 1.954  | 3.227 |
| H    | 8.664  | 4.982  | 11.030 | Cu   | 5.324  | 6.600  | 6.173 | Cu   | 2.928  | 4.435  | 3.227 |
| H    | 7.913  | 3.805  | 9.907  | Cu   | 3.424  | 2.554  | 6.208 | Cu   | 1.086  | 0.382  | 3.213 |
| H    | 6.754  | 5.938  | 9.827  | Cu   | 8.910  | 6.623  | 5.605 | Cu   | 2.811  | 6.902  | 2.562 |
| H    | 8.157  | 6.709  | 9.397  | Cu   | 7.073  | 2.595  | 5.621 | Cu   | 0.949  | 2.833  | 2.540 |
| N    | 7.643  | 5.822  | 9.329  | Cu   | 3.391  | 5.089  | 5.609 | Cu   | 8.336  | 8.446  | 2.535 |
| O    | 10.235 | 5.698  | 8.706  | Cu   | 1.496  | 0.997  | 5.637 | Cu   | 6.503  | 4.404  | 2.557 |
| O    | 10.269 | 3.455  | 9.094  | Cu   | -0.419 | -0.573 | 4.978 | Cu   | 11.981 | 8.467  | 1.951 |
|      |        |        |        | Cu   | 1.389  | 3.454  | 4.959 | Cu   | 10.116 | 4.423  | 1.971 |
|      |        |        |        | Cu   | 5.094  | 0.965  | 4.926 | Cu   | 6.416  | 6.905  | 1.938 |
|      |        |        |        | Cu   | 6.955  | 5.048  | 4.982 | Cu   | 4.590  | 2.848  | 1.954 |
| Cu   | 7.325  | 5.620  | 7.313  | Cu   | 12.379 | 9.110  | 4.365 | Cu   | 10.015 | 6.905  | 1.403 |
| Cu   | 5.482  | 1.620  | 7.213  | Cu   | 10.541 | 5.066  | 4.411 | Cu   | 8.174  | 2.858  | 1.413 |
| Cu   | 1.838  | 4.176  | 7.227  | Cu   | 6.830  | 7.538  | 4.353 | Cu   | 4.467  | 5.351  | 1.414 |
| Cu   | 0.005  | -0.081 | 7.329  | Cu   | 4.982  | 3.488  | 4.370 | Cu   | 2.624  | 1.289  | 1.416 |
| Cu   | 12.762 | 9.734  | 6.724  | Cu   | 10.435 | 7.544  | 3.777 | Cu   | 6.240  | 1.277  | 0.946 |
| Cu   | 10.982 | 5.709  | 6.823  | Cu   | 8.595  | 3.489  | 3.779 | Cu   | 8.071  | 5.343  | 0.917 |
| Cu   | 7.243  | 8.173  | 6.705  | Cu   | 4.896  | 5.977  | 3.773 | Cu   | 0.668  | -0.259 | 0.922 |
| Cu   | 5.372  | 4.097  | 6.739  | Cu   | 3.037  | 1.921  | 3.792 | Cu   | 2.538  | 3.769  | 0.939 |

**Table S5:** Coordinates for the second most stable glycine adsorbed on pure Cu(531)<sup>S</sup>. This configuration is shown in Fig. 1b.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 7.774  | 4.125 | 9.894  | Cu   | 10.759 | 8.142  | 6.189 | Cu   | 8.414  | 5.986  | 3.214 |
| C    | 8.777  | 3.246 | 9.149  | Cu   | 8.945  | 4.122  | 6.104 | Cu   | 6.580  | 1.927  | 3.224 |
| H    | 8.028  | 4.146 | 10.968 | Cu   | 5.234  | 6.619  | 6.250 | Cu   | 2.888  | 4.433  | 3.239 |
| H    | 6.766  | 3.712 | 9.760  | Cu   | 3.396  | 2.529  | 6.203 | Cu   | 1.021  | 0.359  | 3.228 |
| H    | 7.219  | 6.126 | 9.856  | Cu   | 8.833  | 6.618  | 5.608 | Cu   | 2.745  | 6.890  | 2.578 |
| H    | 8.774  | 5.843 | 9.363  | Cu   | 7.025  | 2.576  | 5.603 | Cu   | 0.895  | 2.815  | 2.536 |
| N    | 7.809  | 5.494 | 9.304  | Cu   | 3.310  | 5.067  | 5.649 | Cu   | 8.285  | 8.434  | 2.547 |
| O    | 9.950  | 3.735 | 9.001  | Cu   | 1.452  | 0.986  | 5.641 | Cu   | 6.439  | 4.389  | 2.575 |
| O    | 8.357  | 2.143 | 8.686  | Cu   | -0.502 | -0.596 | 5.024 | Cu   | 11.927 | 8.462  | 1.995 |
|      |        |       |        | Cu   | 1.356  | 3.445  | 4.926 | Cu   | 10.054 | 4.397  | 1.940 |
|      |        |       |        | Cu   | 5.044  | 0.956  | 4.941 | Cu   | 6.362  | 6.896  | 1.971 |
|      |        |       |        | Cu   | 6.878  | 5.051  | 4.995 | Cu   | 4.536  | 2.833  | 1.960 |
| Cu   | 7.294  | 5.623 | 7.321  | Cu   | 12.333 | 9.110  | 4.442 | Cu   | 9.960  | 6.893  | 1.412 |
| Cu   | 5.451  | 1.619 | 7.229  | Cu   | 10.473 | 5.029  | 4.347 | Cu   | 8.107  | 2.842  | 1.407 |
| Cu   | 1.726  | 4.033 | 7.225  | Cu   | 6.766  | 7.531  | 4.383 | Cu   | 4.416  | 5.340  | 1.438 |
| Cu   | -0.082 | 0.100 | 7.354  | Cu   | 4.926  | 3.474  | 4.378 | Cu   | 2.569  | 1.273  | 1.426 |
| Cu   | 12.708 | 9.663 | 6.853  | Cu   | 10.381 | 7.529  | 3.782 | Cu   | 6.193  | 1.260  | 0.941 |
| Cu   | 10.866 | 5.684 | 6.694  | Cu   | 8.525  | 3.468  | 3.770 | Cu   | 7.997  | 5.329  | 0.930 |
| Cu   | 7.195  | 8.164 | 6.739  | Cu   | 4.827  | 5.975  | 3.815 | Cu   | 0.619  | -0.293 | 0.939 |
| Cu   | 5.330  | 4.096 | 6.739  | Cu   | 2.987  | 1.900  | 3.794 | Cu   | 2.484  | 3.777  | 0.952 |

**Table S6:** Coordinates for the third most stable glycine adsorbed on pure Cu(531)<sup>S</sup>. This configuration is shown in Fig. 1c.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 7.961  | 4.126 | 9.891  | Cu   | 10.867 | 8.158  | 6.176 | Cu   | 8.520  | 6.027  | 3.191 |
| C    | 7.682  | 2.834 | 9.094  | Cu   | 9.037  | 4.136  | 6.128 | Cu   | 6.662  | 1.956  | 3.181 |
| C    | 9.418  | 4.549 | 9.884  | Cu   | 5.369  | 6.656  | 6.182 | Cu   | 2.979  | 4.477  | 3.200 |
| H    | 9.574  | 5.446 | 10.503 | Cu   | 3.535  | 2.565  | 6.184 | Cu   | 1.134  | 0.405  | 3.213 |
| H    | 10.054 | 3.737 | 10.260 | Cu   | 8.935  | 6.638  | 5.612 | Cu   | 2.824  | 6.912  | 2.510 |
| H    | 9.729  | 4.782 | 8.848  | Cu   | 7.112  | 2.610  | 5.543 | Cu   | 0.987  | 2.854  | 2.509 |
| H    | 7.630  | 3.931 | 10.929 | Cu   | 3.406  | 5.114  | 5.612 | Cu   | 8.397  | 8.496  | 2.561 |
| H    | 7.218  | 6.061 | 9.868  | Cu   | 1.599  | 1.041  | 5.605 | Cu   | 6.541  | 4.431  | 2.540 |
| H    | 6.131  | 4.918 | 9.367  | Cu   | -0.429 | -0.584 | 4.921 | Cu   | 11.990 | 8.496  | 1.962 |
| N    | 7.115  | 5.210 | 9.304  | Cu   | 1.450  | 3.483  | 4.900 | Cu   | 10.151 | 4.425  | 1.919 |
| O    | 6.446  | 2.577 | 8.894  | Cu   | 5.167  | 1.019  | 4.990 | Cu   | 6.488  | 6.943  | 1.943 |
| O    | 8.677  | 2.148 | 8.714  | Cu   | 7.004  | 5.086  | 4.954 | Cu   | 4.631  | 2.887  | 1.922 |
| Cu   | 7.405  | 5.658 | 7.315  | Cu   | 12.407 | 9.134  | 4.401 | Cu   | 10.041 | 6.937  | 1.393 |
| Cu   | 5.624  | 1.660 | 7.316  | Cu   | 10.565 | 5.060  | 4.332 | Cu   | 8.181  | 2.871  | 1.370 |
| Cu   | 1.845  | 4.058 | 7.188  | Cu   | 6.887  | 7.577  | 4.360 | Cu   | 4.529  | 5.383  | 1.396 |
| Cu   | 0.019  | 0.093 | 7.182  | Cu   | 5.026  | 3.519  | 4.336 | Cu   | 2.687  | 1.324  | 1.405 |
| Cu   | 12.787 | 9.719 | 6.810  | Cu   | 10.463 | 7.562  | 3.776 | Cu   | 6.252  | 1.297  | 0.891 |
| Cu   | 10.974 | 5.682 | 6.694  | Cu   | 8.617  | 3.505  | 3.737 | Cu   | 8.101  | 5.354  | 0.904 |
| Cu   | 7.328  | 8.202 | 6.731  | Cu   | 4.937  | 6.015  | 3.770 | Cu   | 0.741  | -0.247 | 0.930 |
| Cu   | 5.426  | 4.160 | 6.656  | Cu   | 3.101  | 1.955  | 3.769 | Cu   | 2.574  | 3.837  | 0.920 |

**Table S7:** Coordinates for the most stable D-alanine adsorbed on pure Cu(531)<sup>S</sup>. This configuration is shown in Fig. 2a.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.456  | 4.729  | 9.951  | Cu   | 10.833 | 8.194  | 6.182 | Cu   | 8.478  | 5.995  | 3.205 |
| C    | 9.800  | 4.637  | 9.210  | Cu   | 9.014  | 4.107  | 6.142 | Cu   | 6.637  | 1.953  | 3.227 |
| C    | 7.667  | 3.429  | 9.897  | Cu   | 5.325  | 6.601  | 6.170 | Cu   | 2.928  | 4.437  | 3.231 |
| H    | 6.713  | 3.531  | 10.440 | Cu   | 3.425  | 2.556  | 6.209 | Cu   | 1.086  | 0.382  | 3.213 |
| H    | 8.252  | 2.615  | 10.344 | Cu   | 8.911  | 6.624  | 5.605 | Cu   | 2.809  | 6.899  | 2.561 |
| H    | 7.451  | 3.165  | 8.846  | Cu   | 7.074  | 2.596  | 5.620 | Cu   | 0.947  | 2.834  | 2.542 |
| H    | 8.671  | 4.992  | 11.004 | Cu   | 3.392  | 5.090  | 5.611 | Cu   | 8.335  | 8.447  | 2.536 |
| H    | 6.791  | 5.963  | 9.822  | Cu   | 1.498  | 1.002  | 5.634 | Cu   | 6.503  | 4.402  | 2.556 |
| H    | 8.211  | 6.700  | 9.374  | Cu   | -0.419 | -0.573 | 4.975 | Cu   | 11.977 | 8.467  | 1.953 |
| N    | 7.671  | 5.828  | 9.313  | Cu   | 1.388  | 3.457  | 4.960 | Cu   | 10.118 | 4.421  | 1.972 |
| O    | 10.243 | 5.724  | 8.719  | Cu   | 5.094  | 0.966  | 4.927 | Cu   | 6.419  | 6.903  | 1.940 |
| O    | 10.333 | 3.485  | 9.096  | Cu   | 6.955  | 5.048  | 4.980 | Cu   | 4.588  | 2.849  | 1.958 |
| Cu   | 7.326  | 5.627  | 7.307  | Cu   | 12.377 | 9.111  | 4.366 | Cu   | 10.013 | 6.906  | 1.404 |
| Cu   | 5.481  | 1.621  | 7.213  | Cu   | 10.542 | 5.066  | 4.414 | Cu   | 8.174  | 2.857  | 1.413 |
| Cu   | 1.840  | 4.179  | 7.228  | Cu   | 6.831  | 7.539  | 4.354 | Cu   | 4.469  | 5.349  | 1.415 |
| Cu   | 0.008  | -0.072 | 7.319  | Cu   | 4.983  | 3.489  | 4.373 | Cu   | 2.620  | 1.290  | 1.417 |
| Cu   | 12.765 | 9.737  | 6.724  | Cu   | 10.433 | 7.543  | 3.778 | Cu   | 6.239  | 1.281  | 0.946 |
| Cu   | 10.981 | 5.719  | 6.826  | Cu   | 8.595  | 3.489  | 3.780 | Cu   | 8.072  | 5.339  | 0.918 |
| Cu   | 7.241  | 8.175  | 6.705  | Cu   | 4.896  | 5.977  | 3.772 | Cu   | 0.670  | -0.264 | 0.924 |
| Cu   | 5.374  | 4.100  | 6.741  | Cu   | 3.036  | 1.922  | 3.793 | Cu   | 2.536  | 3.772  | 0.944 |

**Table S8:** Coordinates for the most stable L-alanine adsorbed on pure Cu(531)<sup>S</sup>. This configuration is shown in Fig. 2b.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 7.973  | 4.101 | 9.882  | Cu   | 7.328  | 8.222  | 6.744 | Cu   | 3.122  | 1.990  | 3.780 |
| C    | 7.634  | 2.799 | 9.126  | Cu   | 5.438  | 4.178  | 6.674 | Cu   | 8.540  | 6.062  | 3.212 |
| C    | 9.438  | 4.541 | 9.755  | Cu   | 10.895 | 8.197  | 6.188 | Cu   | 6.688  | 1.990  | 3.202 |
| H    | 9.620  | 5.407 | 10.413 | Cu   | 9.068  | 4.163  | 6.165 | Cu   | 3.004  | 4.511  | 3.217 |
| H    | 10.018 | 2.712 | 9.681  | Cu   | 5.387  | 6.675  | 6.198 | Cu   | 1.152  | 0.440  | 3.230 |
| H    | 9.587  | 4.883 | 8.704  | Cu   | 3.543  | 2.592  | 6.193 | Cu   | 2.851  | 6.950  | 2.550 |
| H    | 7.737  | 3.914 | 10.947 | Cu   | 8.953  | 6.670  | 5.641 | Cu   | 1.009  | 2.889  | 2.531 |
| H    | 7.193  | 6.024 | 9.932  | Cu   | 7.134  | 2.638  | 5.573 | Cu   | 8.415  | 8.527  | 2.571 |
| H    | 6.135  | 4.876 | 9.390  | Cu   | 3.426  | 5.143  | 5.626 | Cu   | 6.564  | 4.463  | 2.560 |
| N    | 7.113  | 5.190 | 9.339  | Cu   | 1.614  | 1.071  | 5.611 | Cu   | 12.020 | 8.528  | 1.979 |
| O    | 6.400  | 2.592 | 8.905  | Cu   | -0.398 | -0.543 | 4.966 | Cu   | 10.176 | 4.459  | 1.941 |
| O    | 8.596  | 2.026 | 8.799  | Cu   | 1.471  | 3.519  | 4.916 | Cu   | 6.508  | 6.972  | 1.957 |
| O    | 10.376 | 3.532 | 10.106 | Cu   | 5.181  | 1.045  | 4.997 | Cu   | 4.656  | 2.916  | 1.937 |
|      |        |       |        | Cu   | 7.028  | 5.113  | 4.978 | Cu   | 10.065 | 6.968  | 1.413 |
|      |        |       |        | Cu   | 12.432 | 9.171  | 4.419 | Cu   | 8.211  | 2.903  | 1.396 |
| Cu   | 7.403  | 5.678 | 7.344  | Cu   | 10.581 | 5.097  | 4.351 | Cu   | 4.547  | 5.411  | 1.419 |
| Cu   | 5.610  | 1.662 | 7.318  | Cu   | 6.905  | 7.608  | 4.372 | Cu   | 2.700  | 1.352  | 1.423 |
| Cu   | 1.871  | 4.098 | 7.206  | Cu   | 5.050  | 3.549  | 4.351 | Cu   | 6.284  | 1.328  | 0.912 |
| Cu   | 0.077  | 0.127 | 7.238  | Cu   | 10.483 | 7.598  | 3.792 | Cu   | 8.127  | 5.384  | 0.925 |
| Cu   | 12.827 | 9.767 | 6.831  | Cu   | 8.641  | 3.542  | 3.767 | Cu   | 0.757  | -0.223 | 0.949 |
| Cu   | 11.005 | 5.720 | 6.705  | Cu   | 4.960  | 6.050  | 3.789 | Cu   | 2.597  | 3.860  | 0.938 |

**Table S9:** Coordinates for the most stable D- $\mu_3$ -serine adsorbed on pure Cu(531)<sup>S</sup>. This configuration is shown in Fig. 2c.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.447  | 4.658  | 9.919  | Cu   | 7.249  | 8.182  | 6.743 | Cu   | 3.041  | 1.924  | 3.841 |
| C    | 9.826  | 4.588  | 9.254  | Cu   | 5.377  | 4.113  | 6.766 | Cu   | 8.488  | 5.990  | 3.241 |
| C    | 7.665  | 3.356  | 9.681  | Cu   | 10.827 | 8.199  | 6.237 | Cu   | 6.640  | 1.951  | 3.271 |
| H    | 5.769  | 3.580  | 9.217  | Cu   | 9.026  | 4.104  | 6.185 | Cu   | 2.930  | 4.432  | 3.275 |
| H    | 8.116  | 2.553  | 10.282 | Cu   | 5.338  | 6.602  | 6.194 | Cu   | 1.093  | 0.376  | 3.259 |
| H    | 7.750  | 3.082  | 8.611  | Cu   | 3.427  | 2.568  | 6.253 | Cu   | 2.815  | 6.893  | 2.608 |
| H    | 8.569  | 4.817  | 11.007 | Cu   | 8.918  | 6.626  | 5.640 | Cu   | 0.953  | 2.829  | 2.595 |
| H    | 6.820  | 5.913  | 9.839  | Cu   | 7.077  | 2.597  | 5.669 | Cu   | 8.344  | 8.444  | 2.582 |
| H    | 8.265  | 6.650  | 9.431  | Cu   | 3.393  | 5.094  | 5.650 | Cu   | 6.511  | 4.393  | 2.586 |
| N    | 7.701  | 5.798  | 9.325  | Cu   | 1.502  | 1.005  | 5.677 | Cu   | 11.987 | 8.458  | 1.999 |
| O    | 10.285 | 5.676  | 8.780  | Cu   | -0.412 | -0.573 | 5.018 | Cu   | 10.128 | 4.411  | 2.015 |
| O    | 10.361 | 3.434  | 9.151  | Cu   | 1.387  | 3.462  | 5.009 | Cu   | 6.430  | 6.893  | 1.981 |
| O    | 6.292  | 3.507  | 10.049 | Cu   | 5.101  | 0.976  | 4.982 | Cu   | 4.593  | 2.836  | 1.992 |
|      |        |        |        | Cu   | 6.967  | 5.045  | 5.009 | Cu   | 10.023 | 6.897  | 1.450 |
|      |        |        |        | Cu   | 12.377 | 9.110  | 4.411 | Cu   | 8.185  | 2.847  | 1.457 |
| Cu   | 7.336  | 5.636  | 7.333  | Cu   | 10.547 | 5.066  | 4.457 | Cu   | 4.470  | 5.337  | 1.459 |
| Cu   | 5.478  | 1.650  | 7.276  | Cu   | 6.844  | 7.540  | 4.392 | Cu   | 2.623  | 1.279  | 1.468 |
| Cu   | 1.841  | 4.184  | 7.278  | Cu   | 4.990  | 3.490  | 4.402 | Cu   | 6.252  | 1.269  | 0.989 |
| Cu   | 0.030  | -0.097 | 7.366  | Cu   | 10.436 | 7.547  | 3.823 | Cu   | 8.084  | 5.329  | 0.954 |
| Cu   | 12.772 | 9.736  | 6.763  | Cu   | 8.601  | 3.483  | 3.823 | Cu   | 0.677  | -0.280 | 0.969 |
| Cu   | 10.983 | 5.714  | 6.875  | Cu   | 4.904  | 5.973  | 3.808 | Cu   | 2.539  | 3.757  | 0.987 |

**Table S10:** Coordinates for the most stable L- $\mu_3$ -serine adsorbed on pure Cu(531)<sup>S</sup>. This configuration is shown in Fig. 2d.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.480  | 5.036  | 9.773  | Cu   | 7.423  | 8.071 | 6.696 | Cu   | 3.195  | 1.834 | 3.780 |
| C    | 4.185  | 5.522  | 9.073  | Cu   | 5.505  | 4.015 | 6.697 | Cu   | 8.631  | 5.913 | 3.221 |
| C    | 5.732  | 3.530  | 9.678  | Cu   | 10.992 | 8.032 | 6.227 | Cu   | 6.764  | 1.842 | 3.171 |
| H    | 4.821  | 3.032  | 10.058 | Cu   | 9.159  | 4.032 | 6.214 | Cu   | 3.070  | 4.331 | 3.170 |
| H    | 6.571  | 3.280  | 10.362 | Cu   | 5.483  | 6.511 | 6.087 | Cu   | 1.242  | 0.294 | 3.203 |
| H    | 5.321  | 5.266  | 10.846 | Cu   | 3.587  | 2.419 | 6.157 | Cu   | 2.946  | 6.794 | 2.529 |
| H    | 7.409  | 5.758  | 9.964  | Cu   | 9.045  | 6.493 | 5.675 | Cu   | 1.114  | 2.760 | 2.580 |
| H    | 6.347  | 6.817  | 9.260  | Cu   | 7.221  | 2.465 | 5.523 | Cu   | 8.496  | 8.374 | 2.540 |
| H    | 6.647  | 5.832  | 9.280  | Cu   | 3.540  | 4.991 | 5.517 | Cu   | 6.642  | 4.305 | 2.530 |
| N    | 4.130  | 6.782  | 8.869  | Cu   | 1.658  | 0.884 | 5.621 | Cu   | 12.103 | 8.380 | 1.931 |
| O    | 3.281  | 4.663  | 8.841  | Cu   | 3.394  | 7.457 | 4.930 | Cu   | 10.286 | 4.322 | 1.956 |
| O    | 6.065  | 3.114  | 8.379  | Cu   | 1.573  | 3.398 | 5.018 | Cu   | 6.585  | 6.817 | 1.920 |
|      |        |        |        | Cu   | 8.973  | 8.991 | 4.975 | Cu   | 4.716  | 2.767 | 1.928 |
|      |        |        |        | Cu   | 7.114  | 4.942 | 4.977 | Cu   | 10.167 | 6.825 | 1.418 |
|      |        |        |        | Cu   | 12.513 | 8.993 | 4.338 | Cu   | 8.319  | 2.760 | 1.387 |
| Cu   | 7.421  | 5.557  | 7.368  | Cu   | 10.681 | 4.963 | 4.382 | Cu   | 4.610  | 5.247 | 1.370 |
| Cu   | 5.678  | 1.509  | 7.296  | Cu   | 6.999  | 7.452 | 4.333 | Cu   | 2.764  | 1.207 | 1.405 |
| Cu   | 2.085  | 4.122  | 7.325  | Cu   | 5.140  | 3.401 | 4.351 | Cu   | 10.054 | 9.320 | 0.891 |
| Cu   | 0.095  | -0.177 | 7.294  | Cu   | 10.574 | 7.444 | 3.801 | Cu   | 8.231  | 5.244 | 0.933 |
| Cu   | 12.885 | 9.650  | 6.660  | Cu   | 8.734  | 3.402 | 3.760 | Cu   | 4.523  | 7.732 | 0.916 |
| Cu   | 11.147 | 5.542  | 6.765  | Cu   | 5.049  | 5.888 | 3.728 | Cu   | 2.656  | 3.686 | 0.889 |

**Table S11:** Coordinates for the most stable D- $\mu_4$ -serine adsorbed on pure Cu(531)<sup>S</sup>. This configuration is shown in Fig. 2e.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.152  | 4.303  | 9.725  | Cu   | 7.329  | 8.297  | 6.802 | Cu   | 3.096  | 2.005  | 3.919 |
| C    | 9.613  | 4.427  | 9.254  | Cu   | 5.530  | 4.202  | 6.974 | Cu   | 8.538  | 6.064  | 3.287 |
| C    | 7.499  | 3.045  | 9.048  | Cu   | 10.866 | 8.254  | 6.295 | Cu   | 6.686  | 2.017  | 3.296 |
| H    | 7.656  | 2.181  | 9.718  | Cu   | 9.064  | 4.172  | 6.197 | Cu   | 2.993  | 4.504  | 3.359 |
| H    | 8.112  | 2.839  | 8.125  | Cu   | 5.414  | 6.687  | 6.253 | Cu   | 1.157  | 0.459  | 3.329 |
| H    | 8.134  | 4.166  | 10.821 | Cu   | 3.494  | 2.648  | 6.303 | Cu   | 2.871  | 6.958  | 2.651 |
| H    | 6.441  | 5.442  | 9.662  | Cu   | 8.976  | 6.712  | 5.659 | Cu   | 1.011  | 2.913  | 2.658 |
| H    | 7.847  | 6.341  | 9.799  | Cu   | 7.133  | 2.634  | 5.641 | Cu   | 8.408  | 8.531  | 2.671 |
| H    | 7.414  | 5.528  | 9.349  | Cu   | 3.502  | 5.148  | 5.758 | Cu   | 6.563  | 4.463  | 2.646 |
| N    | 10.010 | 5.566  | 8.844  | Cu   | 1.533  | 1.085  | 5.775 | Cu   | 12.022 | 8.543  | 2.051 |
| O    | 10.288 | 3.342  | 9.212  | Cu   | -0.355 | -0.512 | 5.070 | Cu   | 10.191 | 4.488  | 2.059 |
| O    | 6.147  | 3.180  | 8.697  | Cu   | 1.418  | 3.519  | 5.088 | Cu   | 6.495  | 6.971  | 2.042 |
|      |        |        |        | Cu   | 5.171  | 1.081  | 5.084 | Cu   | 4.640  | 2.929  | 2.103 |
|      |        |        |        | Cu   | 7.017  | 5.115  | 5.064 | Cu   | 10.067 | 6.984  | 1.500 |
|      |        |        |        | Cu   | 12.444 | 9.161  | 4.464 | Cu   | 8.239  | 2.917  | 1.490 |
| Cu   | 7.457  | 5.841  | 7.355  | Cu   | 10.599 | 5.135  | 4.510 | Cu   | 4.537  | 5.412  | 1.510 |
| Cu   | 5.546  | 1.732  | 7.417  | Cu   | 6.899  | 7.620  | 4.455 | Cu   | 2.694  | 1.364  | 1.539 |
| Cu   | 1.866  | 4.215  | 7.328  | Cu   | 5.066  | 3.589  | 4.541 | Cu   | 6.266  | 1.365  | 1.019 |
| Cu   | 0.074  | -0.060 | 7.444  | Cu   | 10.492 | 7.626  | 3.871 | Cu   | 8.133  | 5.387  | 1.006 |
| Cu   | 12.839 | 9.775  | 6.789  | Cu   | 8.660  | 3.550  | 3.851 | Cu   | 0.747  | -0.207 | 1.036 |
| Cu   | 10.952 | 5.765  | 6.998  | Cu   | 4.961  | 6.050  | 3.864 | Cu   | 2.604  | 3.857  | 1.066 |

**Table S12:** Coordinates for the most stable L- $\mu_4$ -serine adsorbed on pure Cu(531)<sup>S</sup>. This configuration is shown in Fig. 2f.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.027  | 4.106 | 9.822  | Cu   | 7.301  | 8.230  | 6.754 | Cu   | 3.114  | 1.983  | 3.782 |
| C    | 7.607  | 2.775 | 9.142  | Cu   | 5.411  | 4.182  | 6.688 | Cu   | 8.536  | 6.064  | 3.236 |
| C    | 9.451  | 4.656 | 9.618  | Cu   | 10.879 | 8.215  | 6.206 | Cu   | 6.689  | 1.993  | 3.230 |
| H    | 9.661  | 5.390 | 10.412 | Cu   | 9.061  | 4.175  | 6.180 | Cu   | 3.006  | 4.513  | 3.240 |
| H    | 9.952  | 2.386 | 9.466  | Cu   | 5.364  | 6.685  | 6.203 | Cu   | 1.144  | 0.431  | 3.229 |
| H    | 9.480  | 5.183 | 8.647  | Cu   | 3.514  | 2.595  | 6.197 | Cu   | 2.858  | 6.960  | 2.587 |
| H    | 7.870  | 3.920 | 10.903 | Cu   | 8.940  | 6.674  | 5.668 | Cu   | 1.009  | 2.881  | 2.550 |
| H    | 7.180  | 6.004 | 9.938  | Cu   | 7.125  | 2.648  | 5.601 | Cu   | 8.412  | 8.521  | 2.579 |
| H    | 6.142  | 4.816 | 9.417  | Cu   | 3.418  | 5.159  | 5.641 | Cu   | 6.556  | 4.460  | 2.574 |
| N    | 7.103  | 5.173 | 9.342  | Cu   | 1.589  | 1.065  | 5.604 | Cu   | 12.027 | 8.530  | 2.014 |
| O    | 6.363  | 2.654 | 8.915  | Cu   | -0.389 | -0.510 | 5.027 | Cu   | 10.174 | 4.461  | 1.957 |
| O    | 8.483  | 1.874 | 8.916  | Cu   | 1.474  | 3.526  | 4.924 | Cu   | 6.492  | 6.970  | 1.971 |
| S    | -0.236 | 0.333 | 9.611  | Cu   | 5.169  | 1.046  | 5.008 | Cu   | 4.655  | 2.910  | 1.956 |
|      |        |       |        | Cu   | 7.012  | 5.112  | 4.986 | Cu   | 10.073 | 6.968  | 1.435 |
|      |        |       |        | Cu   | 12.435 | 9.183  | 4.443 | Cu   | 8.220  | 2.905  | 1.421 |
| Cu   | 7.351  | 5.684 | 7.335  | Cu   | 10.577 | 5.096  | 4.365 | Cu   | 4.539  | 5.412  | 1.433 |
| Cu   | 5.572  | 1.674 | 7.323  | Cu   | 6.899  | 7.607  | 4.384 | Cu   | 2.695  | 1.341  | 1.425 |
| Cu   | 1.859  | 4.121 | 7.214  | Cu   | 5.041  | 3.546  | 4.371 | Cu   | 6.297  | 1.332  | 0.943 |
| Cu   | 0.109  | 0.156 | 7.340  | Cu   | 10.480 | 7.598  | 3.814 | Cu   | 8.127  | 5.396  | 0.952 |
| Cu   | 12.813 | 9.777 | 6.840  | Cu   | 8.639  | 3.544  | 3.787 | Cu   | 0.739  | -0.227 | 0.949 |
| Cu   | 11.013 | 5.741 | 6.689  | Cu   | 4.951  | 6.051  | 3.804 | Cu   | 2.594  | 3.853  | 0.968 |

**Table S13:** Coordinates for the most stable D- $\mu_3$ -cysteine adsorbed on pure Cu(531)<sup>S</sup>. This configuration is shown in Fig. 2g.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.373  | 4.477  | 9.877  | Cu   | 7.267  | 8.228  | 6.805 | Cu   | 3.049  | 1.955  | 3.878 |
| C    | 9.824  | 4.543  | 9.320  | Cu   | 5.374  | 4.181  | 6.721 | Cu   | 8.500  | 6.019  | 3.286 |
| C    | 7.765  | 3.162  | 9.369  | Cu   | 10.832 | 8.236  | 6.294 | Cu   | 6.640  | 1.966  | 3.289 |
| H    | 5.608  | 4.046  | 8.795  | Cu   | 9.029  | 4.138  | 6.202 | Cu   | 2.933  | 4.456  | 3.290 |
| H    | 8.235  | 2.313  | 9.880  | Cu   | 5.337  | 6.653  | 6.223 | Cu   | 1.113  | 0.410  | 3.307 |
| H    | 7.976  | 3.068  | 8.286  | Cu   | 3.450  | 2.593  | 6.275 | Cu   | 2.819  | 6.908  | 2.626 |
| H    | 8.403  | 4.490  | 10.982 | Cu   | 8.927  | 6.666  | 5.690 | Cu   | 0.952  | 2.852  | 2.623 |
| H    | 6.793  | 5.837  | 9.896  | Cu   | 7.081  | 2.619  | 5.675 | Cu   | 8.363  | 8.493  | 2.670 |
| H    | 8.274  | 6.477  | 9.475  | Cu   | 3.389  | 5.119  | 5.648 | Cu   | 6.519  | 4.415  | 2.611 |
| N    | 7.650  | 5.666  | 9.361  | Cu   | 1.505  | 1.048  | 5.733 | Cu   | 11.969 | 8.480  | 2.024 |
| O    | 10.225 | 5.671  | 8.901  | Cu   | -0.407 | -0.541 | 5.036 | Cu   | 10.139 | 4.428  | 2.052 |
| O    | -0.630 | 0.313  | 9.244  | Cu   | 1.386  | 3.489  | 5.040 | Cu   | 6.466  | 6.925  | 2.024 |
| S    | 5.962  | 2.918  | 9.530  | Cu   | 5.130  | 1.045  | 5.103 | Cu   | 4.598  | 2.874  | 2.015 |
|      |        |        |        | Cu   | 6.980  | 5.077  | 5.020 | Cu   | 10.009 | 6.926  | 1.493 |
|      |        |        |        | Cu   | 12.375 | 9.130  | 4.424 | Cu   | 8.183  | 2.858  | 1.475 |
| Cu   | 7.319  | 5.675  | 7.342  | Cu   | 10.552 | 5.097  | 4.497 | Cu   | 4.492  | 5.365  | 1.478 |
| Cu   | 5.526  | 1.726  | 7.448  | Cu   | 6.860  | 7.582  | 4.448 | Cu   | 2.652  | 1.308  | 1.506 |
| Cu   | 1.850  | 4.200  | 7.294  | Cu   | 4.995  | 3.508  | 4.412 | Cu   | 6.224  | 1.290  | 1.009 |
| Cu   | 0.016  | -0.062 | 7.394  | Cu   | 10.433 | 7.578  | 3.871 | Cu   | 8.099  | 5.337  | 0.995 |
| Cu   | 12.796 | 9.750  | 6.758  | Cu   | 8.607  | 3.504  | 3.839 | Cu   | 0.708  | -0.249 | 1.023 |
| Cu   | 10.960 | 5.755  | 6.938  | Cu   | 4.917  | 6.005  | 3.828 | Cu   | 2.539  | 3.793  | 1.016 |

**Table S14:** Coordinates for the most stable L- $\mu_3$ -cysteine adsorbed on pure Cu(531)<sup>S</sup>. This configuration is shown in Fig. 2h.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.468  | 5.305  | 9.869  | Cu   | 7.407  | 7.987 | 6.692 | Cu   | 3.179  | 1.775 | 3.751 |
| C    | 4.156  | 5.604  | 9.097  | Cu   | 5.450  | 3.933 | 6.674 | Cu   | 8.620  | 5.864 | 3.216 |
| C    | 5.840  | 3.829  | 9.959  | Cu   | 11.005 | 7.974 | 6.206 | Cu   | 6.735  | 1.778 | 3.125 |
| H    | 4.929  | 3.243  | 10.129 | Cu   | 9.145  | 3.985 | 6.170 | Cu   | 3.054  | 4.274 | 3.139 |
| H    | 6.534  | 3.667  | 10.800 | Cu   | 5.466  | 6.455 | 6.073 | Cu   | 1.232  | 0.240 | 3.173 |
| H    | 5.261  | 5.658  | 10.899 | Cu   | 3.574  | 2.334 | 6.148 | Cu   | 2.932  | 6.734 | 2.489 |
| H    | 7.339  | 6.202  | 9.977  | Cu   | 9.026  | 6.437 | 5.695 | Cu   | 1.099  | 2.710 | 2.562 |
| H    | 6.210  | 7.072  | 9.130  | Cu   | 7.210  | 2.392 | 5.447 | Cu   | 8.475  | 8.318 | 2.512 |
| N    | 6.577  | 6.125  | 9.295  | Cu   | 3.530  | 4.933 | 5.482 | Cu   | 6.629  | 4.251 | 2.523 |
| O    | 3.961  | 6.845  | 8.876  | Cu   | 1.649  | 0.827 | 5.588 | Cu   | 12.078 | 8.324 | 1.901 |
| O    | 3.379  | 4.639  | 8.830  | Cu   | 3.382  | 7.400 | 4.891 | Cu   | 10.274 | 4.265 | 1.935 |
| S    | 6.695  | 3.205  | 8.457  | Cu   | 1.576  | 3.350 | 5.001 | Cu   | 6.571  | 6.766 | 1.902 |
|      |        |        |        | Cu   | 8.951  | 8.927 | 4.951 | Cu   | 4.701  | 2.713 | 1.887 |
|      |        |        |        | Cu   | 7.099  | 4.894 | 4.972 | Cu   | 10.149 | 6.769 | 1.403 |
|      |        |        |        | Cu   | 12.503 | 8.939 | 4.298 | Cu   | 8.294  | 2.703 | 1.361 |
| Cu   | 7.348  | 5.418  | 7.445  | Cu   | 10.671 | 4.912 | 4.365 | Cu   | 4.606  | 5.192 | 1.347 |
| Cu   | 5.695  | 1.483  | 7.259  | Cu   | 6.984  | 7.395 | 4.318 | Cu   | 2.747  | 1.160 | 1.371 |
| Cu   | 2.129  | 4.087  | 7.318  | Cu   | 5.114  | 3.335 | 4.316 | Cu   | 10.026 | 9.251 | 0.848 |
| Cu   | 0.082  | -0.188 | 7.241  | Cu   | 10.555 | 7.389 | 3.790 | Cu   | 8.216  | 5.190 | 0.925 |
| Cu   | 12.876 | 9.603  | 6.622  | Cu   | 8.721  | 3.351 | 3.727 | Cu   | 4.512  | 7.681 | 0.886 |
| Cu   | 11.150 | 5.499  | 6.741  | Cu   | 5.036  | 5.833 | 3.706 | Cu   | 2.639  | 3.640 | 0.858 |

**Table S15:** Coordinates for the most stable D- $\mu_4$ -cysteine adsorbed on pure Cu(531)<sup>S</sup>. This configuration is shown in Fig. 2i.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.326  | 4.436  | 9.806  | Cu   | 7.271  | 8.231  | 6.789 | Cu   | 3.067  | 1.964  | 3.899 |
| C    | 9.780  | 4.484  | 9.283  | Cu   | 5.431  | 4.168  | 6.990 | Cu   | 8.499  | 6.023  | 3.294 |
| C    | 7.651  | 3.170  | 9.225  | Cu   | 10.853 | 8.223  | 6.282 | Cu   | 6.646  | 1.980  | 3.302 |
| H    | 7.944  | 2.304  | 9.831  | Cu   | 9.050  | 4.138  | 6.204 | Cu   | 2.954  | 4.464  | 3.323 |
| H    | 8.049  | 3.009  | 8.203  | Cu   | 5.376  | 6.624  | 6.231 | Cu   | 1.122  | 0.420  | 3.306 |
| H    | 8.338  | 4.374  | 10.910 | Cu   | 3.454  | 2.590  | 6.288 | Cu   | 2.837  | 6.921  | 2.634 |
| H    | 6.718  | 5.737  | 9.816  | Cu   | 8.950  | 6.672  | 5.674 | Cu   | 0.977  | 2.870  | 2.633 |
| H    | 8.209  | 6.483  | 9.649  | Cu   | 7.097  | 2.607  | 5.674 | Cu   | 8.373  | 8.496  | 2.663 |
| N    | 7.639  | 5.676  | 9.369  | Cu   | 3.451  | 5.103  | 5.708 | Cu   | 6.528  | 4.428  | 2.652 |
| O    | 10.211 | 5.605  | 8.863  | Cu   | 1.510  | 1.035  | 5.739 | Cu   | 11.981 | 8.501  | 2.034 |
| O    | 10.400 | 3.370  | 9.220  | Cu   | -0.384 | -0.549 | 5.053 | Cu   | 10.144 | 4.448  | 2.054 |
| S    | 5.824  | 3.194  | 9.050  | Cu   | 1.402  | 3.487  | 5.062 | Cu   | 6.460  | 6.942  | 2.033 |
|      |        |        |        | Cu   | 5.135  | 1.031  | 5.077 | Cu   | 4.609  | 2.899  | 2.080 |
|      |        |        |        | Cu   | 6.981  | 5.063  | 5.075 | Cu   | 10.020 | 6.944  | 1.495 |
|      |        |        |        | Cu   | 12.403 | 9.130  | 4.443 | Cu   | 8.192  | 2.881  | 1.492 |
| Cu   | 7.417  | 5.767  | 7.362  | Cu   | 10.571 | 5.100  | 4.497 | Cu   | 4.511  | 5.383  | 1.492 |
| Cu   | 5.520  | 1.648  | 7.418  | Cu   | 6.866  | 7.575  | 4.442 | Cu   | 2.669  | 1.334  | 1.517 |
| Cu   | 1.861  | 4.194  | 7.317  | Cu   | 5.031  | 3.543  | 4.529 | Cu   | 6.225  | 1.323  | 1.017 |
| Cu   | 0.064  | -0.102 | 7.419  | Cu   | 10.456 | 7.583  | 3.863 | Cu   | 8.086  | 5.355  | 1.006 |
| Cu   | 12.816 | 9.742  | 6.774  | Cu   | 8.621  | 3.508  | 3.856 | Cu   | 0.714  | -0.230 | 1.015 |
| Cu   | 10.973 | 5.738  | 6.954  | Cu   | 4.926  | 6.005  | 3.849 | Cu   | 2.573  | 3.821  | 1.035 |

**Table S16:** Coordinates for the most stable L- $\mu_4$ -cysteine adsorbed on pure Cu(531)<sup>S</sup>. This configuration is shown in Fig. 2j.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.435  | 5.161  | 9.920  | Cu   | 7.437  | 8.058 | 6.668 | Cu   | 3.200  | 1.818 | 3.740 |
| C    | 4.177  | 5.565  | 9.115  | Cu   | 5.550  | 3.977 | 6.620 | Cu   | 8.662  | 5.910 | 3.149 |
| C    | 5.746  | 3.675  | 9.927  | Cu   | 11.038 | 8.020 | 6.190 | Cu   | 6.809  | 1.855 | 3.153 |
| H    | 4.861  | 3.098  | 10.222 | Cu   | 9.196  | 4.018 | 6.168 | Cu   | 3.090  | 4.328 | 3.147 |
| H    | 6.578  | 3.453  | 10.613 | Cu   | 5.480  | 6.497 | 6.058 | Cu   | 1.254  | 0.281 | 3.165 |
| H    | 6.054  | 3.353  | 8.912  | Cu   | 3.622  | 2.416 | 6.131 | Cu   | 2.967  | 6.793 | 2.501 |
| H    | 5.218  | 5.483  | 10.958 | Cu   | 9.092  | 6.502 | 5.568 | Cu   | 1.135  | 2.758 | 2.545 |
| H    | 7.366  | 5.874  | 10.096 | Cu   | 7.242  | 2.473 | 5.537 | Cu   | 8.503  | 8.357 | 2.469 |
| H    | 6.315  | 6.929  | 9.367  | Cu   | 3.555  | 4.981 | 5.488 | Cu   | 6.670  | 4.301 | 2.462 |
| N    | 6.601  | 5.943  | 9.416  | Cu   | 1.680  | 0.877 | 5.590 | Cu   | 12.140 | 8.387 | 1.902 |
| O    | 4.078  | 6.816  | 8.878  | Cu   | 3.422  | 7.443 | 4.905 | Cu   | 10.304 | 4.326 | 1.907 |
| O    | 3.344  | 4.653  | 8.824  | Cu   | 1.594  | 3.389 | 4.989 | Cu   | 6.596  | 6.802 | 1.867 |
|      |        |        |        | Cu   | 8.970  | 8.963 | 4.869 | Cu   | 4.730  | 2.756 | 1.889 |
|      |        |        |        | Cu   | 7.146  | 4.931 | 4.876 | Cu   | 10.205 | 6.820 | 1.360 |
|      |        |        |        | Cu   | 12.534 | 8.998 | 4.322 | Cu   | 8.358  | 2.773 | 1.340 |
| Pd   | 7.463  | 5.532  | 7.366  | Cu   | 10.707 | 4.950 | 4.338 | Cu   | 4.625  | 5.242 | 1.336 |
| Cu   | 5.685  | 1.489  | 7.145  | Cu   | 7.011  | 7.438 | 4.294 | Cu   | 2.767  | 1.198 | 1.364 |
| Cu   | 2.134  | 4.126  | 7.306  | Cu   | 5.157  | 3.380 | 4.288 | Cu   | 10.097 | 9.330 | 0.881 |
| Cu   | 0.115  | -0.179 | 7.273  | Cu   | 10.607 | 7.443 | 3.743 | Cu   | 8.259  | 5.255 | 0.857 |
| Cu   | 12.907 | 9.649  | 6.653  | Cu   | 8.768  | 3.393 | 3.726 | Cu   | 4.532  | 7.725 | 0.876 |
| Cu   | 11.158 | 5.536  | 6.727  | Cu   | 5.070  | 5.878 | 3.693 | Cu   | 2.672  | 3.683 | 0.860 |

**Table S17:** Coordinates for the most stable D-alanine adsorbed on Pd-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 7.984  | 4.102 | 10.055 | Cu   | 7.161  | 8.165  | 6.715 | Cu   | 2.936  | 1.901  | 3.733 |
| C    | 8.885  | 3.209 | 9.187  | Cu   | 5.273  | 4.103  | 6.690 | Cu   | 8.369  | 5.976  | 3.142 |
| C    | 6.547  | 3.625 | 10.140 | Cu   | 10.709 | 8.145  | 6.137 | Cu   | 6.537  | 1.928  | 3.180 |
| H    | 5.937  | 4.328 | 10.732 | Cu   | 8.912  | 4.109  | 6.069 | Cu   | 2.844  | 4.434  | 3.194 |
| H    | 6.497  | 2.630 | 10.602 | Cu   | 5.189  | 6.618  | 6.172 | Cu   | 0.977  | 0.354  | 3.172 |
| H    | 6.118  | 3.560 | 9.123  | Cu   | 3.352  | 2.530  | 6.147 | Cu   | 2.695  | 6.885  | 2.526 |
| H    | 8.432  | 4.140 | 11.066 | Cu   | 8.799  | 6.620  | 5.524 | Cu   | 0.846  | 2.809  | 2.481 |
| H    | 7.533  | 6.128 | 10.043 | Cu   | 6.979  | 2.586  | 5.557 | Cu   | 8.233  | 8.430  | 2.499 |
| H    | 9.015  | 5.765 | 9.388  | Cu   | 3.258  | 5.075  | 5.598 | Cu   | 6.392  | 4.378  | 2.497 |
| N    | 8.034  | 5.463 | 9.444  | Cu   | 1.419  | 0.984  | 5.579 | Cu   | 11.876 | 8.461  | 1.955 |
| O    | 10.077 | 3.646 | 9.012  | Cu   | -0.550 | -0.589 | 4.974 | Cu   | 10.006 | 4.390  | 1.874 |
| O    | 8.382  | 2.168 | 8.670  | Cu   | 1.298  | 3.445  | 4.872 | Cu   | 6.318  | 6.884  | 1.912 |
|      |        |       |        | Cu   | 4.991  | 0.960  | 4.894 | Cu   | 4.485  | 2.828  | 1.913 |
|      |        |       |        | Cu   | 6.827  | 5.044  | 4.899 | Cu   | 9.908  | 6.886  | 1.351 |
|      |        |       |        | Cu   | 12.285 | 9.113  | 4.403 | Cu   | 8.062  | 2.837  | 1.351 |
| Pd   | 7.263  | 5.617 | 7.357  | Cu   | 10.424 | 5.021  | 4.291 | Cu   | 4.372  | 5.335  | 1.379 |
| Cu   | 5.410  | 1.632 | 7.177  | Cu   | 6.726  | 7.525  | 4.336 | Cu   | 2.518  | 1.265  | 1.367 |
| Cu   | 1.680  | 4.039 | 7.165  | Cu   | 4.884  | 3.476  | 4.330 | Cu   | 6.141  | 1.259  | 0.899 |
| Cu   | -0.086 | 0.084 | 7.300  | Cu   | 10.327 | 7.528  | 3.722 | Cu   | 7.946  | 5.319  | 0.851 |
| Cu   | 12.650 | 9.680 | 6.820  | Cu   | 8.481  | 3.470  | 3.719 | Cu   | 0.574  | -0.307 | 0.884 |
| Cu   | 10.820 | 5.674 | 6.642  | Cu   | 4.777  | 5.978  | 3.757 | Cu   | 2.437  | 3.782  | 0.910 |

**Table S18:** Coordinates for the most stable L-alanine adsorbed on Pd-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.118  | 3.908 | 9.919  | Cu   | 7.289  | 8.273  | 6.768 | Cu   | 3.097  | 2.030  | 3.776 |
| C    | 7.680  | 2.621 | 9.185  | Cu   | 5.405  | 4.221  | 6.705 | Cu   | 8.513  | 6.108  | 3.198 |
| C    | 9.554  | 4.408 | 9.627  | Cu   | 10.872 | 8.256  | 6.169 | Cu   | 6.674  | 2.044  | 3.221 |
| H    | 9.929  | 4.978 | 10.493 | Cu   | 9.052  | 4.207  | 6.165 | Cu   | 2.993  | 4.557  | 3.211 |
| H    | 9.929  | 2.527 | 9.249  | Cu   | 5.324  | 6.736  | 6.206 | Cu   | 1.130  | 0.489  | 3.223 |
| H    | 9.495  | 5.088 | 8.754  | Cu   | 3.528  | 2.629  | 6.195 | Cu   | 2.839  | 7.012  | 2.565 |
| H    | 8.044  | 3.652 | 10.995 | Cu   | 8.920  | 6.731  | 5.607 | Cu   | 0.991  | 2.932  | 2.518 |
| H    | 7.248  | 5.771 | 10.233 | Cu   | 7.114  | 2.695  | 5.597 | Cu   | 8.392  | 8.571  | 2.579 |
| H    | 6.217  | 4.612 | 9.635  | Cu   | 3.411  | 5.176  | 5.608 | Cu   | 6.539  | 4.508  | 2.549 |
| N    | 7.169  | 4.992 | 9.573  | Cu   | 1.572  | 1.119  | 5.615 | Cu   | 12.011 | 8.580  | 1.982 |
| O    | 6.441  | 2.480 | 8.974  | Cu   | -0.405 | -0.468 | 5.012 | Cu   | 10.145 | 4.515  | 1.932 |
| O    | 12.285 | 9.880 | 8.892  | Cu   | 1.451  | 3.565  | 4.899 | Cu   | 6.477  | 7.023  | 1.960 |
| O    | -0.572 | 0.239 | 9.339  | Cu   | 5.152  | 1.094  | 5.002 | Cu   | 4.638  | 2.968  | 1.947 |
|      |        |       |        | Cu   | 6.988  | 5.163  | 4.945 | Cu   | 10.039 | 7.018  | 1.403 |
|      |        |       |        | Cu   | 12.425 | 9.225  | 4.412 | Cu   | 8.196  | 2.958  | 1.401 |
| Pd   | 7.365  | 5.716 | 7.428  | Cu   | 10.556 | 5.142  | 4.343 | Cu   | 4.528  | 5.471  | 1.409 |
| Cu   | 5.584  | 1.697 | 7.325  | Cu   | 6.875  | 7.653  | 4.389 | Cu   | 2.688  | 1.396  | 1.411 |
| Cu   | 1.846  | 4.139 | 7.188  | Cu   | 5.035  | 3.594  | 4.366 | Cu   | 6.268  | 1.386  | 0.935 |
| Cu   | 0.082  | 0.228 | 7.327  | Cu   | 10.462 | 7.644  | 3.780 | Cu   | 8.089  | 5.441  | 0.907 |
| Cu   | 12.818 | 9.795 | 6.799  | Cu   | 8.623  | 3.593  | 3.775 | Cu   | 0.730  | -0.168 | 0.942 |
| Cu   | 10.966 | 5.797 | 6.678  | Cu   | 4.930  | 6.104  | 3.792 | Cu   | 2.587  | 3.907  | 0.937 |

**Table S19:** Coordinates for the most stable D- $\mu_3$ -serine adsorbed on Pd-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 9.299  | 5.968  | 9.844  | Cu   | 7.109  | 8.028 | 6.710 | Cu   | 2.963  | 1.769 | 3.780 |
| C    | 10.208 | 7.011  | 9.146  | Cu   | 5.318  | 3.897 | 6.788 | Cu   | 8.359  | 5.824 | 3.181 |
| C    | 9.550  | 4.464  | 9.568  | Cu   | 10.788 | 8.031 | 6.040 | Cu   | 6.535  | 1.788 | 3.235 |
| H    | 0.321  | 1.840  | 9.123  | Cu   | 8.897  | 3.957 | 6.149 | Cu   | 2.867  | 4.295 | 3.209 |
| H    | 9.250  | 3.875  | 10.450 | Cu   | 5.153  | 6.439 | 6.225 | Cu   | 1.001  | 0.223 | 3.190 |
| H    | 8.898  | 4.175  | 8.719  | Cu   | 3.384  | 2.381 | 6.271 | Cu   | 2.717  | 6.761 | 2.545 |
| H    | 9.469  | 6.156  | 10.923 | Cu   | 8.807  | 6.500 | 5.544 | Cu   | 0.873  | 2.672 | 2.506 |
| H    | 7.249  | 5.854  | 10.181 | Cu   | 6.959  | 2.420 | 5.638 | Cu   | 8.244  | 8.287 | 2.569 |
| H    | 7.764  | 7.275  | 9.490  | Cu   | 3.252  | 4.872 | 5.677 | Cu   | 6.399  | 4.252 | 2.569 |
| N    | 7.888  | 6.255  | 9.488  | Cu   | 1.441  | 0.859 | 5.579 | Cu   | 11.890 | 8.304 | 1.936 |
| O    | 9.719  | 8.149  | 8.930  | Cu   | 3.180  | 7.401 | 4.992 | Cu   | 10.006 | 4.252 | 1.903 |
| O    | 11.428 | 6.639  | 8.924  | Cu   | 1.358  | 3.317 | 4.926 | Cu   | 6.325  | 6.753 | 1.947 |
| O    | -0.171 | 0.971  | 9.240  | Cu   | 4.993  | 0.844 | 4.976 | Cu   | 4.508  | 2.699 | 1.963 |
|      |        |        |        | Cu   | 6.829  | 4.892 | 4.981 | Cu   | 9.903  | 6.734 | 1.377 |
|      |        |        |        | Cu   | 12.315 | 8.965 | 4.340 | Cu   | 8.047  | 2.699 | 1.410 |
| Pd   | 7.270  | 5.554  | 7.411  | Cu   | 10.427 | 4.880 | 4.290 | Cu   | 4.396  | 5.205 | 1.407 |
| Cu   | 5.486  | 1.279  | 7.344  | Cu   | 6.719  | 7.368 | 4.368 | Cu   | 2.558  | 1.130 | 1.396 |
| Cu   | 1.615  | 3.960  | 7.310  | Cu   | 4.887  | 3.341 | 4.396 | Cu   | 9.820  | 9.221 | 0.953 |
| Cu   | -0.090 | -0.038 | 7.316  | Cu   | 10.340 | 7.370 | 3.726 | Cu   | 7.936  | 5.180 | 0.887 |
| Cu   | 12.711 | 9.598  | 6.715  | Cu   | 8.481  | 3.330 | 3.778 | Cu   | 4.294  | 7.696 | 0.907 |
| Cu   | 10.815 | 5.517  | 6.566  | Cu   | 4.774  | 5.832 | 3.805 | Cu   | 2.468  | 3.622 | 0.925 |

**Table S20:** Coordinates for the most stable L- $\mu_3$ -serine adsorbed on Pd-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.376  | 5.018  | 9.833  | Cu   | 7.465  | 8.080 | 6.699 | Cu   | 3.211  | 1.831 | 3.771 |
| C    | 4.116  | 5.524  | 9.092  | Cu   | 5.527  | 4.047 | 6.703 | Cu   | 8.655  | 5.913 | 3.184 |
| C    | 5.636  | 3.514  | 9.696  | Cu   | 11.004 | 8.049 | 6.207 | Cu   | 6.789  | 1.851 | 3.161 |
| H    | 4.722  | 3.002  | 10.049 | Cu   | 9.194  | 4.030 | 6.175 | Cu   | 3.091  | 4.328 | 3.166 |
| H    | 6.464  | 3.252  | 10.389 | Cu   | 5.500  | 6.518 | 6.094 | Cu   | 1.269  | 0.288 | 3.193 |
| H    | 5.154  | 5.189  | 10.907 | Cu   | 3.615  | 2.432 | 6.142 | Cu   | 2.975  | 6.791 | 2.518 |
| H    | 7.285  | 5.744  | 10.147 | Cu   | 9.090  | 6.512 | 5.590 | Cu   | 1.139  | 2.756 | 2.563 |
| H    | 6.248  | 6.823  | 9.427  | Cu   | 7.241  | 2.483 | 5.518 | Cu   | 8.515  | 8.373 | 2.527 |
| N    | 6.550  | 5.841  | 9.440  | Cu   | 3.553  | 4.993 | 5.511 | Cu   | 6.667  | 4.301 | 2.502 |
| O    | 4.083  | 6.780  | 8.869  | Cu   | 1.684  | 0.892 | 5.624 | Cu   | 12.132 | 8.380 | 1.915 |
| O    | 3.207  | 4.675  | 8.842  | Cu   | 3.424  | 7.455 | 4.923 | Cu   | 10.311 | 4.319 | 1.929 |
| O    | 5.992  | 3.115  | 8.396  | Cu   | 1.580  | 3.400 | 5.001 | Cu   | 6.605  | 6.811 | 1.907 |
|      |        |        |        | Cu   | 8.991  | 9.004 | 4.955 | Cu   | 4.733  | 2.764 | 1.919 |
|      |        |        |        | Cu   | 7.136  | 4.941 | 4.924 | Cu   | 10.194 | 6.821 | 1.390 |
|      |        |        |        | Cu   | 12.535 | 8.999 | 4.329 | Cu   | 8.351  | 2.759 | 1.367 |
| Pd   | 7.524  | 5.593  | 7.421  | Cu   | 10.710 | 4.957 | 4.353 | Cu   | 4.633  | 5.245 | 1.363 |
| Cu   | 5.711  | 1.527  | 7.283  | Cu   | 7.024  | 7.452 | 4.329 | Cu   | 2.786  | 1.203 | 1.388 |
| Cu   | 2.074  | 4.117  | 7.305  | Cu   | 5.166  | 3.406 | 4.344 | Cu   | 10.076 | 9.318 | 0.887 |
| Cu   | 0.103  | -0.171 | 7.293  | Cu   | 10.601 | 7.452 | 3.764 | Cu   | 8.254  | 5.238 | 0.898 |
| Cu   | 12.898 | 9.656  | 6.654  | Cu   | 8.765  | 3.397 | 3.738 | Cu   | 4.547  | 7.725 | 0.899 |
| Cu   | 11.142 | 5.550  | 6.748  | Cu   | 5.073  | 5.891 | 3.726 | Cu   | 2.680  | 3.683 | 0.876 |

**Table S21:** Coordinates for the most stable D- $\mu_4$ -serine adsorbed on Pd-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 9.424  | 6.105  | 9.826  | Cu   | 7.091  | 7.990 | 6.686 | Cu   | 2.898  | 1.737 | 3.792 |
| C    | 10.179 | 7.279  | 9.162  | Cu   | 5.287  | 3.881 | 6.757 | Cu   | 8.331  | 5.785 | 3.166 |
| C    | 10.068 | 4.734  | 9.599  | Cu   | 10.708 | 7.991 | 6.039 | Cu   | 6.478  | 1.753 | 3.199 |
| H    | -0.015 | 1.642  | 10.079 | Cu   | 8.823  | 3.887 | 6.124 | Cu   | 2.793  | 4.253 | 3.223 |
| H    | 9.452  | 3.978  | 10.128 | Cu   | 5.155  | 6.381 | 6.190 | Cu   | 0.952  | 0.180 | 3.180 |
| H    | 9.511  | 6.297  | 10.916 | Cu   | 3.311  | 2.375 | 6.271 | Cu   | 2.669  | 6.701 | 2.497 |
| H    | 7.446  | 5.591  | 10.116 | Cu   | 8.784  | 6.456 | 5.527 | Cu   | 0.819  | 2.645 | 2.532 |
| H    | 7.680  | 7.111  | 9.490  | Cu   | 6.898  | 2.385 | 5.583 | Cu   | 8.201  | 8.259 | 2.553 |
| N    | 7.991  | 6.133  | 9.438  | Cu   | 3.204  | 4.852 | 5.678 | Cu   | 6.366  | 4.205 | 2.549 |
| O    | 9.483  | 8.318  | 8.922  | Cu   | 1.381  | 0.802 | 5.583 | Cu   | 11.819 | 8.274 | 1.913 |
| O    | 11.430 | 7.132  | 8.971  | Cu   | 3.131  | 7.325 | 4.932 | Cu   | 9.978  | 4.218 | 1.917 |
| O    | 10.178 | 4.377  | 8.241  | Cu   | 1.275  | 3.276 | 4.986 | Cu   | 6.293  | 6.708 | 1.928 |
|      |        |        |        | Cu   | 8.631  | 8.939 | 4.959 | Cu   | 4.444  | 2.664 | 1.965 |
|      |        |        |        | Cu   | 6.799  | 4.858 | 4.952 | Cu   | 9.858  | 6.706 | 1.366 |
|      |        |        |        | Cu   | 12.244 | 8.919 | 4.308 | Cu   | 8.007  | 2.663 | 1.390 |
| Pd   | 7.276  | 5.509  | 7.399  | Cu   | 10.402 | 4.853 | 4.354 | Cu   | 4.353  | 5.157 | 1.396 |
| Cu   | 5.440  | 1.339  | 7.320  | Cu   | 6.688  | 7.335 | 4.345 | Cu   | 2.508  | 1.099 | 1.403 |
| Cu   | 1.571  | 4.006  | 7.364  | Cu   | 4.831  | 3.312 | 4.380 | Cu   | 9.754  | 9.201 | 0.913 |
| Cu   | -0.147 | -0.272 | 7.274  | Cu   | 10.289 | 7.338 | 3.721 | Cu   | 7.910  | 5.132 | 0.872 |
| Cu   | 12.614 | 9.544  | 6.660  | Cu   | 8.457  | 3.292 | 3.760 | Cu   | 4.259  | 7.656 | 0.891 |
| Cu   | 10.798 | 5.499  | 6.711  | Cu   | 4.743  | 5.781 | 3.774 | Cu   | 2.402  | 3.593 | 0.933 |

**Table S22:** Coordinates for the most stable L- $\mu_4$ -serine adsorbed on Pd-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.067  | 3.984  | 9.929  | Cu   | 7.300  | 8.271  | 6.749 | Cu   | 3.106  | 2.010  | 3.760 |
| C    | 7.632  | 2.701  | 9.175  | Cu   | 5.404  | 4.221  | 6.690 | Cu   | 8.523  | 6.083  | 3.185 |
| C    | 9.476  | 4.559  | 9.686  | Cu   | 10.869 | 8.241  | 6.179 | Cu   | 6.680  | 2.026  | 3.213 |
| H    | 9.709  | 5.271  | 10.493 | Cu   | 9.065  | 4.192  | 6.164 | Cu   | 2.998  | 4.537  | 3.213 |
| H    | -1.093 | -0.813 | 9.414  | Cu   | 5.340  | 6.720  | 6.173 | Cu   | 1.138  | 0.462  | 3.207 |
| H    | 9.459  | 5.114  | 8.731  | Cu   | 3.526  | 2.625  | 6.177 | Cu   | 2.846  | 6.986  | 2.562 |
| H    | 7.978  | 3.719  | 11.002 | Cu   | 8.936  | 6.711  | 5.593 | Cu   | 1.000  | 2.908  | 2.515 |
| H    | 7.206  | 5.857  | 10.214 | Cu   | 7.116  | 2.685  | 5.591 | Cu   | 8.399  | 8.546  | 2.568 |
| H    | 6.161  | 4.695  | 9.631  | Cu   | 3.407  | 5.176  | 5.610 | Cu   | 6.548  | 4.485  | 2.537 |
| N    | 7.117  | 5.065  | 9.571  | Cu   | 1.585  | 1.102  | 5.587 | Cu   | 12.019 | 8.556  | 1.985 |
| O    | 6.389  | 2.587  | 8.953  | Cu   | -0.399 | -0.483 | 5.007 | Cu   | 10.153 | 4.487  | 1.924 |
| O    | 12.203 | 9.934  | 8.880  | Cu   | 1.455  | 3.550  | 4.896 | Cu   | 6.483  | 6.998  | 1.945 |
| S    | -0.200 | 0.252  | 9.596  | Cu   | 5.163  | 1.081  | 4.995 | Cu   | 4.647  | 2.940  | 1.933 |
|      |        |        |        | Cu   | 7.002  | 5.141  | 4.929 | Cu   | 10.052 | 6.987  | 1.396 |
|      |        |        |        | Cu   | 12.425 | 9.210  | 4.420 | Cu   | 8.206  | 2.931  | 1.391 |
| Pd   | 7.367  | 5.721  | 7.406  | Cu   | 10.568 | 5.120  | 4.336 | Cu   | 4.535  | 5.445  | 1.401 |
| Cu   | 5.581  | 1.708  | 7.321  | Cu   | 6.890  | 7.632  | 4.372 | Cu   | 2.689  | 1.370  | 1.397 |
| Cu   | 1.849  | 4.132  | 7.187  | Cu   | 5.040  | 3.580  | 4.356 | Cu   | 6.280  | 1.352  | 0.930 |
| Cu   | 0.115  | 0.190  | 7.326  | Cu   | 10.470 | 7.626  | 3.775 | Cu   | 8.099  | 5.414  | 0.892 |
| Cu   | 12.807 | 9.795  | 6.817  | Cu   | 8.632  | 3.570  | 3.768 | Cu   | 0.729  | -0.199 | 0.927 |
| Cu   | 10.982 | 5.769  | 6.674  | Cu   | 4.938  | 6.081  | 3.779 | Cu   | 2.594  | 3.887  | 0.936 |

**Table S23:** Coordinates for the most stable D- $\mu_3$ -cysteine adsorbed on Pd-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 5.134  | 4.961 | 9.816  | Cu   | 7.457  | 8.296  | 6.714 | Cu   | 3.252  | 2.039  | 3.755 |
| C    | 4.540  | 3.622 | 9.278  | Cu   | 5.589  | 4.247  | 6.579 | Cu   | 8.695  | 6.141  | 3.209 |
| C    | 4.285  | 6.080 | 9.219  | Cu   | 11.074 | 8.285  | 6.294 | Cu   | 6.841  | 2.070  | 3.207 |
| H    | 3.285  | 6.067 | 9.672  | Cu   | 9.185  | 4.231  | 6.242 | Cu   | 3.114  | 4.553  | 3.213 |
| H    | 6.066  | 7.575 | 8.687  | Cu   | 5.489  | 6.778  | 6.103 | Cu   | 1.275  | 0.497  | 3.227 |
| H    | 4.158  | 5.881 | 8.139  | Cu   | 3.705  | 2.648  | 6.091 | Cu   | 2.990  | 7.021  | 2.585 |
| H    | 5.018  | 4.952 | 10.916 | Cu   | 9.075  | 6.733  | 5.662 | Cu   | 1.155  | 2.965  | 2.608 |
| H    | 7.066  | 5.605 | 10.184 | Cu   | 7.271  | 2.683  | 5.632 | Cu   | 8.553  | 8.594  | 2.554 |
| H    | 6.943  | 4.090 | 9.507  | Cu   | 3.551  | 5.200  | 5.585 | Cu   | 6.696  | 4.527  | 2.504 |
| N    | 6.577  | 5.051 | 9.475  | Cu   | 1.736  | 1.166  | 5.601 | Cu   | 12.167 | 8.602  | 1.972 |
| O    | 5.377  | 2.669 | 9.117  | Cu   | -0.255 | -0.433 | 5.000 | Cu   | 10.327 | 4.543  | 1.974 |
| O    | 3.297  | 3.581 | 9.036  | Cu   | 1.609  | 3.626  | 5.028 | Cu   | 6.623  | 7.028  | 1.946 |
| S    | 4.880  | 7.797 | 9.368  | Cu   | 5.363  | 1.100  | 5.003 | Cu   | 4.770  | 2.972  | 1.909 |
|      |        |       |        | Cu   | 7.180  | 5.182  | 4.920 | Cu   | 10.235 | 7.045  | 1.430 |
|      |        |       |        | Cu   | 12.555 | 9.228  | 4.391 | Cu   | 8.387  | 2.990  | 1.400 |
| Pd   | 7.428  | 5.756 | 7.467  | Cu   | 10.711 | 5.171  | 4.407 | Cu   | 4.643  | 5.465  | 1.401 |
| Cu   | 5.684  | 1.749 | 7.352  | Cu   | 7.053  | 7.681  | 4.353 | Cu   | 2.795  | 1.400  | 1.408 |
| Cu   | 2.159  | 4.102 | 7.389  | Cu   | 5.200  | 3.604  | 4.295 | Cu   | 6.437  | 1.424  | 0.928 |
| Cu   | 0.183  | 0.275 | 7.324  | Cu   | 10.628 | 7.663  | 3.830 | Cu   | 8.291  | 5.483  | 0.921 |
| Cu   | 12.998 | 9.836 | 6.750  | Cu   | 8.776  | 3.615  | 3.793 | Cu   | 0.858  | -0.176 | 0.941 |
| Cu   | 11.130 | 5.829 | 6.757  | Cu   | 5.085  | 6.103  | 3.764 | Cu   | 2.694  | 3.886  | 0.934 |

**Table S24:** Coordinates for the most stable L- $\mu_3$ -cysteine adsorbed on Pd-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.392  | 5.308  | 9.913  | Cu   | 7.459  | 7.993 | 6.701 | Cu   | 3.189  | 1.763 | 3.747 |
| C    | 4.101  | 5.591  | 9.106  | Cu   | 5.450  | 3.956 | 6.671 | Cu   | 8.637  | 5.850 | 3.187 |
| C    | 5.813  | 3.843  | 9.967  | Cu   | 11.011 | 7.983 | 6.195 | Cu   | 6.754  | 1.777 | 3.116 |
| H    | 4.921  | 3.225  | 10.126 | Cu   | 9.151  | 3.985 | 6.138 | Cu   | 3.063  | 4.262 | 3.138 |
| H    | 6.512  | 3.688  | 10.806 | Cu   | 5.466  | 6.465 | 6.079 | Cu   | 1.250  | 0.226 | 3.170 |
| H    | 5.128  | 5.600  | 10.951 | Cu   | 3.596  | 2.344 | 6.130 | Cu   | 2.950  | 6.718 | 2.482 |
| H    | 7.221  | 6.275  | 10.128 | Cu   | 9.066  | 6.456 | 5.610 | Cu   | 1.116  | 2.696 | 2.554 |
| H    | 6.088  | 7.125  | 9.259  | Cu   | 7.226  | 2.405 | 5.438 | Cu   | 8.488  | 8.307 | 2.512 |
| N    | 6.481  | 6.192  | 9.424  | Cu   | 3.531  | 4.937 | 5.472 | Cu   | 6.647  | 4.235 | 2.497 |
| O    | 3.892  | 6.826  | 8.865  | Cu   | 1.669  | 0.829 | 5.596 | Cu   | 12.099 | 8.315 | 1.886 |
| O    | 3.344  | 4.612  | 8.828  | Cu   | 3.395  | 7.399 | 4.887 | Cu   | 10.292 | 4.253 | 1.914 |
| S    | 6.693  | 3.240  | 8.464  | Cu   | 1.576  | 3.344 | 4.992 | Cu   | 6.587  | 6.752 | 1.904 |
|      |        |        |        | Cu   | 8.970  | 8.940 | 4.939 | Cu   | 4.711  | 2.697 | 1.879 |
|      |        |        |        | Cu   | 7.104  | 4.883 | 4.921 | Cu   | 10.169 | 6.754 | 1.382 |
|      |        |        |        | Cu   | 12.512 | 8.938 | 4.291 | Cu   | 8.316  | 2.694 | 1.341 |
| Pd   | 7.437  | 5.478  | 7.468  | Cu   | 10.691 | 4.900 | 4.346 | Cu   | 4.624  | 5.177 | 1.348 |
| Cu   | 5.726  | 1.519  | 7.250  | Cu   | 7.007  | 7.389 | 4.329 | Cu   | 2.767  | 1.140 | 1.364 |
| Cu   | 2.121  | 4.076  | 7.306  | Cu   | 5.128  | 3.336 | 4.304 | Cu   | 10.038 | 9.236 | 0.849 |
| Cu   | 0.073  | -0.180 | 7.240  | Cu   | 10.574 | 7.389 | 3.761 | Cu   | 8.232  | 5.179 | 0.897 |
| Cu   | 12.879 | 9.601  | 6.621  | Cu   | 8.744  | 3.339 | 3.703 | Cu   | 4.532  | 7.661 | 0.881 |
| Cu   | 11.141 | 5.500  | 6.729  | Cu   | 5.052  | 5.834 | 3.709 | Cu   | 2.655  | 3.619 | 0.856 |

**Table S25:** Coordinates for the most stable D- $\mu_4$ -cysteine adsorbed on Pd-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.335  | 4.384  | 9.894  | Cu   | 7.276  | 8.274  | 6.778 | Cu   | 3.066  | 1.964  | 3.890 |
| C    | 9.766  | 4.458  | 9.309  | Cu   | 5.405  | 4.182  | 7.000 | Cu   | 8.512  | 6.027  | 3.255 |
| C    | 7.640  | 3.149  | 9.254  | Cu   | 10.858 | 8.237  | 6.261 | Cu   | 6.653  | 1.999  | 3.291 |
| H    | 7.916  | 2.255  | 9.827  | Cu   | 9.053  | 4.145  | 6.185 | Cu   | 2.949  | 4.468  | 3.311 |
| H    | 8.041  | 3.025  | 8.229  | Cu   | 5.343  | 6.644  | 6.195 | Cu   | 1.129  | 0.419  | 3.291 |
| H    | 8.397  | 4.236  | 10.988 | Cu   | 3.465  | 2.610  | 6.272 | Cu   | 2.843  | 6.929  | 2.619 |
| H    | 6.714  | 5.667  | 10.022 | Cu   | 8.976  | 6.700  | 5.608 | Cu   | 0.986  | 2.875  | 2.629 |
| H    | 8.195  | 6.443  | 9.880  | Cu   | 7.094  | 2.635  | 5.668 | Cu   | 8.374  | 8.496  | 2.642 |
| N    | 7.635  | 5.642  | 9.574  | Cu   | 3.437  | 5.116  | 5.688 | Cu   | 6.527  | 4.424  | 2.591 |
| O    | 10.172 | 5.583  | 8.876  | Cu   | 1.507  | 1.056  | 5.737 | Cu   | 11.996 | 8.513  | 2.014 |
| O    | 10.390 | 3.347  | 9.213  | Cu   | -0.390 | -0.533 | 5.038 | Cu   | 10.161 | 4.452  | 2.033 |
| S    | 5.812  | 3.178  | 9.060  | Cu   | 1.390  | 3.496  | 5.056 | Cu   | 6.468  | 6.934  | 2.005 |
|      |        |        |        | Cu   | 5.142  | 1.052  | 5.056 | Cu   | 4.600  | 2.897  | 2.069 |
|      |        |        |        | Cu   | 6.970  | 5.071  | 4.993 | Cu   | 10.035 | 6.951  | 1.470 |
|      |        |        |        | Cu   | 12.403 | 9.146  | 4.428 | Cu   | 8.208  | 2.889  | 1.467 |
| Pd   | 7.431  | 5.808  | 7.380  | Cu   | 10.576 | 5.104  | 4.480 | Cu   | 4.500  | 5.381  | 1.469 |
| Cu   | 5.538  | 1.663  | 7.407  | Cu   | 6.873  | 7.576  | 4.430 | Cu   | 2.668  | 1.327  | 1.503 |
| Cu   | 1.858  | 4.204  | 7.307  | Cu   | 5.031  | 3.557  | 4.510 | Cu   | 6.235  | 1.341  | 1.010 |
| Cu   | 0.054  | -0.091 | 7.412  | Cu   | 10.467 | 7.599  | 3.828 | Cu   | 8.106  | 5.356  | 0.966 |
| Cu   | 12.810 | 9.757  | 6.765  | Cu   | 8.626  | 3.519  | 3.834 | Cu   | 0.720  | -0.241 | 0.994 |
| Cu   | 10.948 | 5.749  | 6.968  | Cu   | 4.923  | 6.014  | 3.820 | Cu   | 2.568  | 3.811  | 1.017 |

**Table S26:** Coordinates for the most stable L- $\mu_4$ -cysteine adsorbed on Pd-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 7.955  | 4.053 | 9.985  | Cu   | 7.342  | 8.243  | 6.720 | Cu   | 3.106  | 1.963  | 3.747 |
| C    | 7.697  | 2.798 | 9.126  | Cu   | 5.437  | 4.195  | 6.646 | Cu   | 8.531  | 6.030  | 3.139 |
| C    | 9.399  | 4.523 | 9.950  | Cu   | 10.856 | 8.181  | 6.147 | Cu   | 6.672  | 1.968  | 3.156 |
| H    | 9.533  | 5.424 | 10.569 | Cu   | 9.035  | 4.138  | 6.096 | Cu   | 2.978  | 4.480  | 3.173 |
| H    | 10.069 | 3.734 | 10.314 | Cu   | 5.337  | 6.693  | 6.162 | Cu   | 1.141  | 0.419  | 3.204 |
| H    | 9.678  | 4.771 | 8.909  | Cu   | 3.585  | 2.576  | 6.145 | Cu   | 2.831  | 6.919  | 2.501 |
| H    | 7.670  | 3.791 | 11.023 | Cu   | 8.936  | 6.670  | 5.522 | Cu   | 1.005  | 2.870  | 2.499 |
| H    | 7.138  | 5.956 | 10.084 | Cu   | 7.113  | 2.632  | 5.521 | Cu   | 8.397  | 8.497  | 2.539 |
| H    | 6.089  | 4.801 | 9.518  | Cu   | 3.404  | 5.126  | 5.573 | Cu   | 6.549  | 4.430  | 2.486 |
| N    | 7.060  | 5.130 | 9.483  | Cu   | 1.600  | 1.080  | 5.608 | Cu   | 12.004 | 8.505  | 1.927 |
| O    | 6.466  | 2.523 | 8.917  | Cu   | -0.428 | -0.566 | 4.913 | Cu   | 10.163 | 4.442  | 1.892 |
| O    | 8.704  | 2.154 | 8.704  | Cu   | 1.449  | 3.500  | 4.887 | Cu   | 6.488  | 6.940  | 1.923 |
|      |        |       |        | Cu   | 5.176  | 1.040  | 4.962 | Cu   | 4.629  | 2.890  | 1.897 |
|      |        |       |        | Cu   | 6.999  | 5.103  | 4.878 | Cu   | 10.057 | 6.941  | 1.357 |
|      |        |       |        | Cu   | 12.410 | 9.142  | 4.385 | Cu   | 8.200  | 2.879  | 1.340 |
| Pd   | 7.420  | 5.708 | 7.356  | Cu   | 10.573 | 5.071  | 4.312 | Cu   | 4.528  | 5.384  | 1.369 |
| Pd   | 1.853  | 4.028 | 7.315  | Cu   | 6.882  | 7.590  | 4.350 | Cu   | 2.686  | 1.329  | 1.378 |
| Cu   | 5.648  | 1.690 | 7.304  | Cu   | 5.041  | 3.537  | 4.309 | Cu   | 6.258  | 1.305  | 0.874 |
| Cu   | 0.009  | 0.135 | 7.178  | Cu   | 10.475 | 7.578  | 3.736 | Cu   | 8.103  | 5.363  | 0.850 |
| Cu   | 12.786 | 9.745 | 6.793  | Cu   | 8.627  | 3.514  | 3.708 | Cu   | 0.745  | -0.249 | 0.920 |
| Cu   | 10.911 | 5.699 | 6.688  | Cu   | 4.931  | 6.026  | 3.748 | Cu   | 2.575  | 3.832  | 0.882 |

**Table S27:** Coordinates for the most stable D-alanine adsorbed on Pd-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 7.361  | 4.105 | 10.066 | Cu   | 7.087  | 8.279  | 6.752 | Cu   | 2.871  | 2.019  | 3.778 |
| C    | 7.311  | 2.839 | 9.184  | Cu   | 5.193  | 4.231  | 6.724 | Cu   | 8.294  | 6.080  | 3.190 |
| C    | 5.990  | 4.668 | 10.398 | Cu   | 10.645 | 8.239  | 6.178 | Cu   | 6.441  | 2.023  | 3.207 |
| H    | 6.088  | 5.584 | 11.003 | Cu   | 8.825  | 4.200  | 6.127 | Cu   | 2.753  | 4.538  | 3.217 |
| H    | 5.392  | 3.933 | 10.951 | Cu   | 5.126  | 6.721  | 6.195 | Cu   | 0.911  | 0.471  | 3.233 |
| H    | 5.460  | 4.920 | 9.463  | Cu   | 3.338  | 2.624  | 6.183 | Cu   | 2.596  | 6.976  | 2.542 |
| H    | 7.898  | 3.831 | 10.995 | Cu   | 8.732  | 6.735  | 5.564 | Cu   | 0.770  | 2.922  | 2.532 |
| H    | 8.328  | 5.938 | 9.905  | Cu   | 6.871  | 2.689  | 5.578 | Cu   | 8.163  | 8.548  | 2.571 |
| H    | 9.050  | 4.724 | 9.029  | Cu   | 3.174  | 5.194  | 5.624 | Cu   | 6.314  | 4.489  | 2.538 |
| N    | 8.145  | 5.122 | 9.315  | Cu   | 1.372  | 1.127  | 5.622 | Cu   | 11.771 | 8.557  | 1.974 |
| O    | 8.428  | 2.451 | 8.714  | Cu   | -0.656 | -0.504 | 4.953 | Cu   | 9.922  | 4.491  | 1.927 |
| O    | 6.173  | 2.305 | 8.993  | Cu   | 1.226  | 3.560  | 4.925 | Cu   | 6.258  | 6.996  | 1.955 |
|      |        |       |        | Cu   | 4.933  | 1.087  | 4.986 | Cu   | 4.401  | 2.945  | 1.946 |
|      |        |       |        | Cu   | 6.750  | 5.152  | 4.933 | Cu   | 9.818  | 6.993  | 1.394 |
|      |        |       |        | Cu   | 12.184 | 9.207  | 4.436 | Cu   | 7.958  | 2.934  | 1.387 |
| Pd   | 7.206  | 5.752 | 7.389  | Cu   | 10.345 | 5.130  | 4.341 | Cu   | 4.299  | 5.438  | 1.407 |
| Pd   | 1.630  | 4.109 | 7.356  | Cu   | 6.655  | 7.637  | 4.381 | Cu   | 2.459  | 1.383  | 1.408 |
| Cu   | 5.377  | 1.683 | 7.320  | Cu   | 4.803  | 3.593  | 4.363 | Cu   | 6.026  | 1.358  | 0.919 |
| Cu   | -0.181 | 0.184 | 7.215  | Cu   | 10.247 | 7.634  | 3.772 | Cu   | 7.865  | 5.416  | 0.893 |
| Cu   | 12.547 | 9.834 | 6.863  | Cu   | 8.389  | 3.570  | 3.760 | Cu   | 0.511  | -0.196 | 0.956 |
| Cu   | 10.714 | 5.747 | 6.718  | Cu   | 4.695  | 6.085  | 3.782 | Cu   | 2.345  | 3.889  | 0.930 |

**Table S28:** Coordinates for the most stable L-alanine adsorbed on Pd-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.127  | 3.895 | 9.921  | Cu   | 7.285  | 8.273  | 6.773 | Cu   | 3.094  | 2.036  | 3.768 |
| C    | 7.686  | 2.610 | 9.188  | Cu   | 5.392  | 4.226  | 6.710 | Cu   | 8.510  | 6.110  | 3.199 |
| C    | 9.565  | 4.392 | 9.630  | Cu   | 10.861 | 8.263  | 6.163 | Cu   | 6.670  | 2.045  | 3.219 |
| H    | 9.944  | 4.954 | 10.499 | Cu   | 9.052  | 4.204  | 6.161 | Cu   | 2.987  | 4.558  | 3.200 |
| H    | 9.934  | 2.510 | 9.242  | Cu   | 5.326  | 6.739  | 6.206 | Cu   | 1.132  | 0.499  | 3.222 |
| H    | 9.509  | 5.080 | 8.763  | Cu   | 3.545  | 2.617  | 6.176 | Cu   | 2.835  | 7.014  | 2.564 |
| H    | 8.053  | 3.637 | 10.996 | Cu   | 8.910  | 6.735  | 5.602 | Cu   | 0.993  | 2.942  | 2.518 |
| H    | 7.260  | 5.759 | 10.240 | Cu   | 7.105  | 2.699  | 5.597 | Cu   | 8.387  | 8.573  | 2.574 |
| H    | 6.228  | 4.603 | 9.641  | Cu   | 3.412  | 5.190  | 5.587 | Cu   | 6.541  | 4.513  | 2.550 |
| N    | 7.180  | 4.982 | 9.578  | Cu   | 1.572  | 1.133  | 5.619 | Cu   | 12.005 | 8.579  | 1.975 |
| O    | 6.446  | 2.473 | 8.978  | Cu   | -0.400 | -0.459 | 5.002 | Cu   | 10.140 | 4.521  | 1.930 |
| O    | 12.288 | 9.869 | 8.897  | Cu   | 1.453  | 3.575  | 4.900 | Cu   | 6.476  | 7.030  | 1.957 |
| O    | -0.566 | 0.222 | 9.333  | Cu   | 5.148  | 1.096  | 5.000 | Cu   | 4.633  | 2.974  | 1.941 |
|      |        |       |        | Cu   | 6.980  | 5.166  | 4.948 | Cu   | 10.037 | 7.019  | 1.398 |
|      |        |       |        | Cu   | 12.419 | 9.222  | 4.407 | Cu   | 8.191  | 2.960  | 1.401 |
| Pd   | 7.370  | 5.711 | 7.431  | Cu   | 10.559 | 5.152  | 4.336 | Cu   | 4.529  | 5.474  | 1.403 |
| Pd   | 1.862  | 4.121 | 7.333  | Cu   | 6.870  | 7.659  | 4.388 | Cu   | 2.685  | 1.408  | 1.398 |
| Cu   | 5.582  | 1.701 | 7.329  | Cu   | 5.035  | 3.600  | 4.361 | Cu   | 6.261  | 1.385  | 0.933 |
| Cu   | 0.090  | 0.225 | 7.325  | Cu   | 10.459 | 7.648  | 3.777 | Cu   | 8.085  | 5.446  | 0.905 |
| Cu   | 12.818 | 9.819 | 6.784  | Cu   | 8.619  | 3.592  | 3.774 | Cu   | 0.727  | -0.161 | 0.944 |
| Cu   | 10.935 | 5.789 | 6.676  | Cu   | 4.930  | 6.109  | 3.784 | Cu   | 2.579  | 3.909  | 0.918 |

**Table S29:** Coordinates for the most stable D- $\mu_3$ -serine adsorbed on Pd-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y     | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|-------|-------|
| C    | 9.223  | 5.947 | 9.885  | Cu   | 7.114  | 8.018  | 6.707 | Cu   | 2.989  | 1.766 | 3.760 |
| C    | 10.145 | 7.013 | 9.243  | Cu   | 5.306  | 3.900  | 6.771 | Cu   | 8.364  | 5.825 | 3.177 |
| C    | 9.528  | 4.450 | 9.599  | Cu   | 10.811 | 8.026  | 6.059 | Cu   | 6.545  | 1.785 | 3.227 |
| H    | 0.281  | 1.910 | 9.174  | Cu   | 8.918  | 3.965  | 6.145 | Cu   | 2.880  | 4.296 | 3.163 |
| H    | 9.292  | 3.850 | 10.493 | Cu   | 5.151  | 6.453  | 6.220 | Cu   | 1.014  | 0.235 | 3.182 |
| H    | 8.858  | 4.129 | 8.776  | Cu   | 3.436  | 2.356  | 6.230 | Cu   | 2.722  | 6.764 | 2.539 |
| H    | 9.351  | 6.119 | 10.972 | Cu   | 8.814  | 6.495  | 5.543 | Cu   | 0.882  | 2.674 | 2.479 |
| H    | 7.165  | 5.824 | 10.162 | Cu   | 6.972  | 2.414  | 5.654 | Cu   | 8.254  | 8.288 | 2.562 |
| H    | 7.700  | 7.244 | 9.484  | Cu   | 3.291  | 4.882  | 5.587 | Cu   | 6.407  | 4.255 | 2.552 |
| N    | 7.823  | 6.223 | 9.486  | Cu   | 1.460  | 0.878  | 5.569 | Cu   | 11.895 | 8.301 | 1.922 |
| O    | 9.630  | 8.131 | 8.959  | Cu   | -0.501 | -0.699 | 4.981 | Cu   | 10.007 | 4.254 | 1.899 |
| O    | 11.382 | 6.685 | 9.145  | Cu   | 1.377  | 3.320  | 4.874 | Cu   | 6.338  | 6.758 | 1.930 |
| O    | -0.195 | 1.019 | 9.210  | Cu   | 8.715  | 8.948  | 4.976 | Cu   | 4.515  | 2.705 | 1.935 |
|      |        |       |        | Cu   | 6.830  | 4.891  | 4.970 | Cu   | 9.904  | 6.736 | 1.372 |
|      |        |       |        | Cu   | 12.324 | 8.965  | 4.338 | Cu   | 8.053  | 2.699 | 1.402 |
| Pd   | 7.262  | 5.539 | 7.400  | Cu   | 10.440 | 4.889  | 4.283 | Cu   | 4.405  | 5.209 | 1.377 |
| Pd   | 1.719  | 3.938 | 7.365  | Cu   | 6.729  | 7.371  | 4.362 | Cu   | 2.571  | 1.137 | 1.376 |
| Cu   | 5.502  | 1.242 | 7.364  | Cu   | 4.909  | 3.334  | 4.368 | Cu   | 9.825  | 9.217 | 0.942 |
| Cu   | -0.059 | 0.014 | 7.317  | Cu   | 10.352 | 7.377  | 3.726 | Cu   | 7.942  | 5.178 | 0.876 |
| Cu   | 12.757 | 9.606 | 6.716  | Cu   | 8.483  | 3.330  | 3.777 | Cu   | 4.297  | 7.702 | 0.903 |
| Cu   | 10.836 | 5.545 | 6.565  | Cu   | 4.792  | 5.841  | 3.775 | Cu   | 2.467  | 3.624 | 0.882 |

**Table S30:** Coordinates for the most stable L- $\mu_3$ -serine adsorbed on Pd-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.438  | 5.039  | 9.864  | Cu   | 7.468  | 8.082 | 6.692 | Cu   | 3.206  | 1.825 | 3.752 |
| C    | 4.164  | 5.580  | 9.171  | Cu   | 5.509  | 4.072 | 6.709 | Cu   | 8.644  | 5.902 | 3.169 |
| C    | 5.651  | 3.528  | 9.698  | Cu   | 10.954 | 8.051 | 6.169 | Cu   | 6.784  | 1.842 | 3.154 |
| H    | 4.723  | 3.043  | 10.051 | Cu   | 9.183  | 4.006 | 6.167 | Cu   | 3.088  | 4.320 | 3.161 |
| H    | 6.478  | 3.226  | 10.373 | Cu   | 5.494  | 6.530 | 6.102 | Cu   | 1.260  | 0.283 | 3.194 |
| H    | 5.250  | 5.193  | 10.947 | Cu   | 3.616  | 2.429 | 6.121 | Cu   | 2.971  | 6.785 | 2.523 |
| H    | 7.358  | 5.757  | 10.149 | Cu   | 9.073  | 6.502 | 5.561 | Cu   | 1.132  | 2.743 | 2.519 |
| H    | 6.308  | 6.829  | 9.434  | Cu   | 7.235  | 2.479 | 5.511 | Cu   | 8.508  | 8.360 | 2.509 |
| N    | 6.614  | 5.848  | 9.452  | Cu   | 3.537  | 4.994 | 5.520 | Cu   | 6.665  | 4.295 | 2.502 |
| O    | 4.188  | 6.829  | 8.881  | Cu   | 1.674  | 0.903 | 5.629 | Cu   | 12.134 | 8.367 | 1.903 |
| O    | 3.203  | 4.777  | 9.034  | Cu   | 3.413  | 7.454 | 4.933 | Cu   | 10.296 | 4.314 | 1.919 |
| O    | 5.975  | 3.136  | 8.386  | Cu   | 1.548  | 3.379 | 4.934 | Cu   | 6.592  | 6.803 | 1.915 |
|      |        |        |        | Cu   | 8.974  | 9.007 | 4.937 | Cu   | 4.736  | 2.754 | 1.911 |
|      |        |        |        | Cu   | 7.126  | 4.939 | 4.923 | Cu   | 10.188 | 6.808 | 1.365 |
|      |        |        |        | Cu   | 12.528 | 8.991 | 4.327 | Cu   | 8.347  | 2.750 | 1.366 |
| Pd   | 7.536  | 5.596  | 7.415  | Cu   | 10.698 | 4.950 | 4.332 | Cu   | 4.635  | 5.241 | 1.367 |
| Pd   | 1.994  | 4.037  | 7.354  | Cu   | 7.012  | 7.453 | 4.327 | Cu   | 2.785  | 1.195 | 1.371 |
| Cu   | 5.710  | 1.543  | 7.276  | Cu   | 5.162  | 3.405 | 4.342 | Cu   | 10.080 | 9.304 | 0.878 |
| Cu   | 0.089  | -0.172 | 7.311  | Cu   | 10.587 | 7.448 | 3.736 | Cu   | 8.235  | 5.234 | 0.883 |
| Cu   | 12.882 | 9.639  | 6.671  | Cu   | 8.757  | 3.387 | 3.735 | Cu   | 4.539  | 7.727 | 0.900 |
| Cu   | 11.094 | 5.532  | 6.728  | Cu   | 5.059  | 5.883 | 3.739 | Cu   | 2.688  | 3.678 | 0.860 |

**Table S31:** Coordinates for the most stable D- $\mu_4$ -serine adsorbed on Pd-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 9.392  | 6.096  | 9.850  | Cu   | 7.094  | 7.985 | 6.690 | Cu   | 2.911  | 1.729 | 3.775 |
| C    | 10.140 | 7.298  | 9.228  | Cu   | 5.267  | 3.889 | 6.749 | Cu   | 8.326  | 5.779 | 3.169 |
| C    | 10.061 | 4.740  | 9.602  | Cu   | 10.727 | 7.981 | 6.064 | Cu   | 6.482  | 1.744 | 3.197 |
| H    | 11.059 | 4.785  | 10.073 | Cu   | 8.835  | 3.894 | 6.126 | Cu   | 2.797  | 4.246 | 3.185 |
| H    | 9.462  | 3.965  | 10.122 | Cu   | 5.158  | 6.395 | 6.186 | Cu   | 0.953  | 0.190 | 3.180 |
| H    | 9.468  | 6.260  | 10.946 | Cu   | 3.350  | 2.358 | 6.226 | Cu   | 2.664  | 6.696 | 2.498 |
| H    | 7.410  | 5.584  | 10.128 | Cu   | 8.780  | 6.453 | 5.528 | Cu   | 0.816  | 2.640 | 2.510 |
| H    | 7.657  | 7.097  | 9.496  | Cu   | 6.903  | 2.386 | 5.595 | Cu   | 8.202  | 8.254 | 2.548 |
| N    | 7.962  | 6.117  | 9.450  | Cu   | 3.240  | 4.866 | 5.587 | Cu   | 6.366  | 4.202 | 2.541 |
| O    | 9.409  | 8.303  | 8.918  | Cu   | 1.392  | 0.817 | 5.583 | Cu   | 11.816 | 8.263 | 1.909 |
| O    | 11.399 | 7.214  | 9.153  | Cu   | 3.134  | 7.340 | 4.926 | Cu   | 9.967  | 4.214 | 1.920 |
| O    | 10.172 | 4.400  | 8.236  | Cu   | 1.287  | 3.272 | 4.940 | Cu   | 6.296  | 6.709 | 1.921 |
|      |        |        |        | Cu   | 8.651  | 8.925 | 4.958 | Cu   | 4.445  | 2.660 | 1.947 |
|      |        |        |        | Cu   | 6.794  | 4.859 | 4.952 | Cu   | 9.849  | 6.701 | 1.366 |
|      |        |        |        | Cu   | 12.247 | 8.914 | 4.310 | Cu   | 8.004  | 2.657 | 1.389 |
| Pd   | 7.270  | 5.501  | 7.402  | Cu   | 10.405 | 4.856 | 4.354 | Cu   | 4.353  | 5.151 | 1.377 |
| Pd   | 1.692  | 3.988  | 7.412  | Cu   | 6.690  | 7.339 | 4.344 | Cu   | 2.506  | 1.099 | 1.389 |
| Cu   | 5.455  | 1.333  | 7.330  | Cu   | 4.847  | 3.303 | 4.358 | Cu   | 9.754  | 9.193 | 0.908 |
| Cu   | -0.123 | -0.240 | 7.272  | Cu   | 10.291 | 7.337 | 3.727 | Cu   | 7.906  | 5.129 | 0.867 |
| Cu   | 12.641 | 9.553  | 6.660  | Cu   | 8.451  | 3.287 | 3.764 | Cu   | 4.252  | 7.653 | 0.899 |
| Cu   | 10.801 | 5.530  | 6.717  | Cu   | 4.752  | 5.790 | 3.749 | Cu   | 2.396  | 3.585 | 0.901 |

**Table S32:** Coordinates for the most stable L- $\mu_4$ -serine adsorbed on Pd-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.066  | 3.981  | 9.932  | Cu   | 7.300  | 8.270  | 6.750 | Cu   | 3.107  | 2.012  | 3.753 |
| C    | 7.630  | 2.697  | 9.178  | Cu   | 5.396  | 4.225  | 6.693 | Cu   | 8.524  | 6.084  | 3.186 |
| C    | 9.477  | 4.553  | 9.688  | Cu   | 10.863 | 8.247  | 6.174 | Cu   | 6.680  | 2.022  | 3.209 |
| H    | 9.711  | 5.267  | 10.493 | Cu   | 9.065  | 4.186  | 6.159 | Cu   | 2.993  | 4.535  | 3.198 |
| H    | -1.092 | -0.819 | 9.417  | Cu   | 5.340  | 6.723  | 6.176 | Cu   | 1.140  | 0.467  | 3.208 |
| H    | 9.460  | 5.107  | 8.731  | Cu   | 3.548  | 2.612  | 6.158 | Cu   | 2.847  | 6.986  | 2.563 |
| H    | 7.976  | 3.719  | 11.006 | Cu   | 8.927  | 6.714  | 5.586 | Cu   | 1.007  | 2.917  | 2.520 |
| H    | 7.206  | 5.856  | 10.211 | Cu   | 7.114  | 2.684  | 5.589 | Cu   | 8.398  | 8.546  | 2.563 |
| H    | 6.161  | 4.693  | 9.630  | Cu   | 3.410  | 5.184  | 5.590 | Cu   | 6.551  | 4.486  | 2.535 |
| N    | 7.117  | 5.062  | 9.570  | Cu   | 1.585  | 1.115  | 5.595 | Cu   | 12.018 | 8.553  | 1.974 |
| O    | 6.386  | 2.586  | 8.954  | Cu   | -0.395 | -0.477 | 5.004 | Cu   | 10.157 | 4.491  | 1.921 |
| O    | 12.201 | 9.931  | 8.887  | Cu   | 1.460  | 3.559  | 4.903 | Cu   | 6.483  | 6.997  | 1.943 |
| S    | -0.200 | 0.244  | 9.598  | Cu   | 5.163  | 1.079  | 4.988 | Cu   | 4.642  | 2.943  | 1.928 |
|      |        |        |        | Cu   | 6.996  | 5.142  | 4.930 | Cu   | 10.056 | 6.990  | 1.393 |
|      |        |        |        | Cu   | 12.424 | 9.207  | 4.416 | Cu   | 8.208  | 2.931  | 1.389 |
| Pd   | 7.373  | 5.720  | 7.406  | Cu   | 10.571 | 5.125  | 4.332 | Cu   | 4.532  | 5.442  | 1.396 |
| Pd   | 1.867  | 4.106  | 7.337  | Cu   | 6.884  | 7.636  | 4.371 | Cu   | 2.688  | 1.375  | 1.386 |
| Cu   | 5.585  | 1.710  | 7.322  | Cu   | 5.043  | 3.581  | 4.349 | Cu   | 6.277  | 1.356  | 0.925 |
| Cu   | 0.121  | 0.194  | 7.329  | Cu   | 10.471 | 7.628  | 3.775 | Cu   | 8.102  | 5.416  | 0.891 |
| Cu   | 12.812 | 9.812  | 6.808  | Cu   | 8.633  | 3.568  | 3.767 | Cu   | 0.730  | -0.199 | 0.929 |
| Cu   | 10.950 | 5.763  | 6.672  | Cu   | 4.935  | 6.081  | 3.774 | Cu   | 2.583  | 3.878  | 0.917 |

**Table S33:** Coordinates for the most stable D- $\mu_3$ -cysteine adsorbed on Pd-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 5.176  | 4.947 | 9.842  | Cu   | 7.448  | 8.310  | 6.715 | Cu   | 3.247  | 2.050  | 3.756 |
| C    | 4.608  | 3.572 | 9.368  | Cu   | 5.572  | 4.253  | 6.588 | Cu   | 8.688  | 6.142  | 3.201 |
| C    | 4.288  | 6.021 | 9.216  | Cu   | 11.030 | 8.308  | 6.258 | Cu   | 6.837  | 2.070  | 3.201 |
| H    | 3.284  | 5.972 | 9.658  | Cu   | 9.184  | 4.237  | 6.232 | Cu   | 3.119  | 4.555  | 3.192 |
| H    | 6.031  | 7.564 | 8.715  | Cu   | 5.484  | 6.790  | 6.102 | Cu   | 1.276  | 0.508  | 3.226 |
| H    | 4.178  | 5.810 | 8.136  | Cu   | 3.687  | 2.666  | 6.108 | Cu   | 2.992  | 7.025  | 2.582 |
| H    | 5.074  | 4.983 | 10.943 | Cu   | 9.060  | 6.743  | 5.644 | Cu   | 1.154  | 2.969  | 2.577 |
| H    | 7.108  | 5.611 | 10.179 | Cu   | 7.264  | 2.697  | 5.622 | Cu   | 8.549  | 8.598  | 2.549 |
| H    | 6.981  | 4.099 | 9.489  | Cu   | 3.552  | 5.216  | 5.559 | Cu   | 6.700  | 4.529  | 2.503 |
| N    | 6.611  | 5.061 | 9.474  | Cu   | 1.721  | 1.181  | 5.607 | Cu   | 12.167 | 8.599  | 1.963 |
| O    | 5.490  | 2.668 | 9.117  | Cu   | -0.261 | -0.420 | 4.994 | Cu   | 10.322 | 4.549  | 1.965 |
| O    | 3.361  | 3.459 | 9.257  | Cu   | 1.587  | 3.630  | 4.970 | Cu   | 6.621  | 7.033  | 1.941 |
| S    | 4.826  | 7.759 | 9.362  | Cu   | 5.338  | 1.122  | 4.998 | Cu   | 4.772  | 2.978  | 1.901 |
|      |        |       |        | Cu   | 7.166  | 5.186  | 4.916 | Cu   | 10.233 | 7.045  | 1.414 |
|      |        |       |        | Cu   | 12.553 | 9.231  | 4.389 | Cu   | 8.387  | 2.987  | 1.395 |
| Pd   | 7.428  | 5.764 | 7.457  | Cu   | 10.707 | 5.182  | 4.393 | Cu   | 4.649  | 5.471  | 1.392 |
| Pd   | 2.073  | 4.154 | 7.428  | Cu   | 7.045  | 7.692  | 4.352 | Cu   | 2.803  | 1.412  | 1.400 |
| Cu   | 5.688  | 1.764 | 7.358  | Cu   | 5.196  | 3.609  | 4.296 | Cu   | 6.437  | 1.421  | 0.921 |
| Cu   | 0.170  | 0.271 | 7.330  | Cu   | 10.610 | 7.677  | 3.811 | Cu   | 8.284  | 5.483  | 0.910 |
| Cu   | 12.986 | 9.849 | 6.751  | Cu   | 8.773  | 3.617  | 3.788 | Cu   | 0.860  | -0.162 | 0.940 |
| Cu   | 11.094 | 5.831 | 6.749  | Cu   | 5.081  | 6.110  | 3.757 | Cu   | 2.696  | 3.892  | 0.906 |

**Table S34:** Coordinates for the most stable L- $\mu_3$ -cysteine adsorbed on Pd-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.443  | 5.336  | 9.946  | Cu   | 7.464  | 8.002 | 6.695 | Cu   | 3.185  | 1.757 | 3.729 |
| C    | 4.131  | 5.621  | 9.175  | Cu   | 5.430  | 3.976 | 6.682 | Cu   | 8.627  | 5.839 | 3.173 |
| C    | 5.848  | 3.865  | 9.976  | Cu   | 10.953 | 7.989 | 6.150 | Cu   | 6.757  | 1.768 | 3.114 |
| H    | 4.948  | 3.256  | 10.134 | Cu   | 9.142  | 3.966 | 6.140 | Cu   | 3.065  | 4.252 | 3.130 |
| H    | 6.556  | 3.684  | 10.801 | Cu   | 5.455  | 6.475 | 6.088 | Cu   | 1.247  | 0.219 | 3.172 |
| H    | 5.206  | 5.617  | 10.994 | Cu   | 3.597  | 2.345 | 6.109 | Cu   | 2.954  | 6.714 | 2.488 |
| H    | 7.261  | 6.329  | 10.130 | Cu   | 9.044  | 6.445 | 5.582 | Cu   | 1.115  | 2.679 | 2.504 |
| H    | 6.103  | 7.143  | 9.255  | Cu   | 7.227  | 2.400 | 5.435 | Cu   | 8.486  | 8.293 | 2.498 |
| N    | 6.518  | 6.221  | 9.434  | Cu   | 3.515  | 4.931 | 5.478 | Cu   | 6.650  | 4.230 | 2.501 |
| O    | 3.947  | 6.854  | 8.880  | Cu   | 1.659  | 0.840 | 5.605 | Cu   | 12.108 | 8.300 | 1.877 |
| O    | 3.343  | 4.656  | 8.989  | Cu   | 3.387  | 7.399 | 4.899 | Cu   | 10.280 | 4.247 | 1.902 |
| S    | 6.697  | 3.270  | 8.450  | Cu   | 1.541  | 3.320 | 4.915 | Cu   | 6.576  | 6.742 | 1.912 |
|      |        |        |        | Cu   | 8.954  | 8.944 | 4.922 | Cu   | 4.717  | 2.688 | 1.875 |
|      |        |        |        | Cu   | 7.096  | 4.880 | 4.927 | Cu   | 10.169 | 6.739 | 1.357 |
|      |        |        |        | Cu   | 12.510 | 8.926 | 4.291 | Cu   | 8.321  | 2.682 | 1.341 |
| Pd   | 7.440  | 5.495  | 7.471  | Cu   | 10.682 | 4.891 | 4.323 | Cu   | 4.629  | 5.175 | 1.351 |
| Pd   | 2.010  | 3.985  | 7.340  | Cu   | 6.994  | 7.387 | 4.329 | Cu   | 2.775  | 1.132 | 1.347 |
| Cu   | 5.723  | 1.539  | 7.244  | Cu   | 5.128  | 3.330 | 4.305 | Cu   | 10.050 | 9.223 | 0.847 |
| Cu   | 0.060  | -0.179 | 7.259  | Cu   | 10.562 | 7.381 | 3.729 | Cu   | 8.219  | 5.172 | 0.883 |
| Cu   | 12.871 | 9.581  | 6.635  | Cu   | 8.741  | 3.330 | 3.703 | Cu   | 4.530  | 7.665 | 0.882 |
| Cu   | 11.093 | 5.491  | 6.707  | Cu   | 5.040  | 5.821 | 3.724 | Cu   | 2.668  | 3.616 | 0.833 |

**Table S35:** Coordinates for the most stable D- $\mu_4$ -cysteine adsorbed on Pd-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.331  | 4.376  | 9.895  | Cu   | 7.272  | 8.277  | 6.780 | Cu   | 3.067  | 1.965  | 3.882 |
| C    | 9.764  | 4.452  | 9.313  | Cu   | 5.403  | 4.188  | 6.997 | Cu   | 8.512  | 6.023  | 3.254 |
| C    | 7.637  | 3.143  | 9.250  | Cu   | 10.852 | 8.238  | 6.255 | Cu   | 6.653  | 1.993  | 3.289 |
| H    | 7.909  | 2.247  | 9.822  | Cu   | 9.052  | 4.146  | 6.179 | Cu   | 2.952  | 4.466  | 3.296 |
| H    | 8.040  | 3.021  | 8.227  | Cu   | 5.342  | 6.650  | 6.197 | Cu   | 1.131  | 0.422  | 3.292 |
| H    | 8.394  | 4.225  | 10.989 | Cu   | 3.486  | 2.602  | 6.247 | Cu   | 2.841  | 6.929  | 2.623 |
| H    | 6.710  | 5.657  | 10.024 | Cu   | 8.968  | 6.704  | 5.604 | Cu   | 0.992  | 2.882  | 2.630 |
| H    | 8.192  | 6.433  | 9.891  | Cu   | 7.091  | 2.635  | 5.666 | Cu   | 8.373  | 8.493  | 2.635 |
| N    | 7.632  | 5.635  | 9.578  | Cu   | 3.436  | 5.123  | 5.667 | Cu   | 6.531  | 4.425  | 2.592 |
| O    | 10.172 | 5.577  | 8.885  | Cu   | 1.509  | 1.070  | 5.739 | Cu   | 11.999 | 8.509  | 2.014 |
| O    | 10.389 | 3.341  | 9.215  | Cu   | -0.386 | -0.521 | 5.036 | Cu   | 10.159 | 4.452  | 2.035 |
| S    | 5.807  | 3.177  | 9.052  | Cu   | 1.399  | 3.515  | 5.057 | Cu   | 6.468  | 6.935  | 2.008 |
|      |        |        |        | Cu   | 5.143  | 1.051  | 5.049 | Cu   | 4.599  | 2.896  | 2.062 |
|      |        |        |        | Cu   | 6.969  | 5.075  | 4.995 | Cu   | 10.038 | 6.951  | 1.467 |
|      |        |        |        | Cu   | 12.405 | 9.142  | 4.430 | Cu   | 8.208  | 2.889  | 1.465 |
| Pd   | 7.432  | 5.812  | 7.385  | Cu   | 10.581 | 5.111  | 4.474 | Cu   | 4.502  | 5.379  | 1.468 |
| Pd   | 1.888  | 4.190  | 7.458  | Cu   | 6.870  | 7.580  | 4.430 | Cu   | 2.665  | 1.332  | 1.495 |
| Cu   | 5.539  | 1.661  | 7.405  | Cu   | 5.035  | 3.559  | 4.497 | Cu   | 6.241  | 1.338  | 1.009 |
| Cu   | 0.064  | -0.080 | 7.416  | Cu   | 10.466 | 7.600  | 3.826 | Cu   | 8.102  | 5.358  | 0.963 |
| Cu   | 12.812 | 9.780  | 6.756  | Cu   | 8.625  | 3.515  | 3.834 | Cu   | 0.720  | -0.240 | 1.002 |
| Cu   | 10.911 | 5.731  | 6.949  | Cu   | 4.922  | 6.015  | 3.819 | Cu   | 2.562  | 3.810  | 1.000 |

**Table S36:** Coordinates for the most stable L- $\mu_4$ -cysteine adsorbed on Pd-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.445  | 5.158  | 9.900  | Cu   | 7.434  | 8.053 | 6.689 | Cu   | 3.202  | 1.818 | 3.737 |
| C    | 4.177  | 5.565  | 9.111  | Cu   | 5.544  | 3.976 | 6.630 | Cu   | 8.661  | 5.913 | 3.153 |
| C    | 5.749  | 3.673  | 9.930  | Cu   | 11.042 | 8.017 | 6.184 | Cu   | 6.810  | 1.850 | 3.154 |
| H    | 4.857  | 3.108  | 10.230 | Cu   | 9.176  | 4.028 | 6.208 | Cu   | 3.092  | 4.327 | 3.145 |
| H    | 6.576  | 3.454  | 10.624 | Cu   | 5.462  | 6.506 | 6.065 | Cu   | 1.250  | 0.282 | 3.168 |
| H    | 6.059  | 3.332  | 8.923  | Cu   | 3.627  | 2.414 | 6.129 | Cu   | 2.967  | 6.793 | 2.501 |
| H    | 5.255  | 5.503  | 10.935 | Cu   | 9.087  | 6.498 | 5.588 | Cu   | 1.132  | 2.755 | 2.551 |
| H    | 7.388  | 5.866  | 10.033 | Cu   | 7.241  | 2.471 | 5.535 | Cu   | 8.504  | 8.359 | 2.467 |
| H    | 6.322  | 6.922  | 9.327  | Cu   | 3.554  | 4.978 | 5.485 | Cu   | 6.673  | 4.303 | 2.470 |
| N    | 6.609  | 5.936  | 9.369  | Cu   | 1.683  | 0.879 | 5.590 | Cu   | 12.139 | 8.384 | 1.902 |
| O    | 4.079  | 6.817  | 8.881  | Cu   | 3.416  | 7.448 | 4.914 | Cu   | 10.302 | 4.326 | 1.914 |
| O    | 3.341  | 4.655  | 8.828  | Cu   | 1.595  | 3.386 | 4.989 | Cu   | 6.597  | 6.803 | 1.870 |
|      |        |        |        | Cu   | 8.967  | 8.959 | 4.870 | Cu   | 4.734  | 2.756 | 1.888 |
|      |        |        |        | Cu   | 7.146  | 4.937 | 4.874 | Cu   | 10.204 | 6.821 | 1.362 |
|      |        |        |        | Cu   | 12.536 | 8.995 | 4.319 | Cu   | 8.357  | 2.772 | 1.349 |
| Pt   | 7.437  | 5.542  | 7.348  | Cu   | 10.700 | 4.949 | 4.351 | Cu   | 4.628  | 5.242 | 1.337 |
| Cu   | 5.690  | 1.483  | 7.140  | Cu   | 7.006  | 7.444 | 4.292 | Cu   | 2.766  | 1.198 | 1.366 |
| Cu   | 2.134  | 4.120  | 7.306  | Cu   | 5.161  | 3.380 | 4.289 | Cu   | 10.099 | 9.332 | 0.879 |
| Cu   | 0.103  | -0.164 | 7.280  | Cu   | 10.604 | 7.438 | 3.749 | Cu   | 8.259  | 5.253 | 0.858 |
| Cu   | 12.906 | 9.646  | 6.651  | Cu   | 8.765  | 3.393 | 3.735 | Cu   | 4.532  | 7.724 | 0.879 |
| Cu   | 11.170 | 5.537  | 6.736  | Cu   | 5.067  | 5.883 | 3.696 | Cu   | 2.672  | 3.680 | 0.865 |

**Table S37:** Coordinates for the most stable D-alanine adsorbed on Pt-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 7.963  | 4.114 | 10.032 | Cu   | 7.171  | 8.158  | 6.739 | Cu   | 2.942  | 1.900  | 3.738 |
| C    | 8.876  | 3.214 | 9.183  | Cu   | 5.286  | 4.102  | 6.710 | Cu   | 8.373  | 5.976  | 3.147 |
| C    | 6.531  | 3.628 | 10.136 | Cu   | 10.716 | 8.140  | 6.143 | Cu   | 6.539  | 1.924  | 3.182 |
| H    | 5.917  | 4.335 | 10.716 | Cu   | 8.908  | 4.103  | 6.091 | Cu   | 2.850  | 4.430  | 3.193 |
| H    | 6.497  | 2.641 | 10.617 | Cu   | 5.189  | 6.618  | 6.185 | Cu   | 0.979  | 0.353  | 3.176 |
| H    | 6.100  | 3.536 | 9.122  | Cu   | 3.363  | 2.524  | 6.156 | Cu   | 2.699  | 6.886  | 2.530 |
| H    | 8.416  | 4.192 | 11.038 | Cu   | 8.811  | 6.619  | 5.530 | Cu   | 0.850  | 2.808  | 2.488 |
| H    | 7.503  | 6.141 | 9.983  | Cu   | 6.980  | 2.568  | 5.551 | Cu   | 8.238  | 8.430  | 2.502 |
| H    | 8.987  | 5.770 | 9.339  | Cu   | 3.267  | 5.068  | 5.600 | Cu   | 6.396  | 4.379  | 2.504 |
| N    | 8.005  | 5.470 | 9.390  | Cu   | 1.429  | 0.981  | 5.585 | Cu   | 11.878 | 8.460  | 1.958 |
| O    | 10.065 | 3.657 | 9.013  | Cu   | -0.547 | -0.589 | 4.985 | Cu   | 10.011 | 4.389  | 1.880 |
| O    | 8.382  | 2.164 | 8.676  | Cu   | 1.305  | 3.440  | 4.875 | Cu   | 6.321  | 6.883  | 1.914 |
|      |        |       |        | Cu   | 4.991  | 0.955  | 4.899 | Cu   | 4.487  | 2.831  | 1.917 |
|      |        |       |        | Cu   | 6.826  | 5.044  | 4.891 | Cu   | 9.912  | 6.888  | 1.357 |
|      |        |       |        | Cu   | 12.294 | 9.108  | 4.406 | Cu   | 8.065  | 2.838  | 1.360 |
| Pt   | 7.250  | 5.633 | 7.326  | Cu   | 10.425 | 5.016  | 4.298 | Cu   | 4.373  | 5.334  | 1.383 |
| Cu   | 5.418  | 1.629 | 7.180  | Cu   | 6.728  | 7.531  | 4.334 | Cu   | 2.524  | 1.262  | 1.371 |
| Cu   | 1.689  | 4.037 | 7.166  | Cu   | 4.890  | 3.475  | 4.339 | Cu   | 6.142  | 1.263  | 0.900 |
| Cu   | -0.084 | 0.081 | 7.308  | Cu   | 10.331 | 7.525  | 3.731 | Cu   | 7.953  | 5.319  | 0.855 |
| Cu   | 12.655 | 9.675 | 6.821  | Cu   | 8.485  | 3.467  | 3.730 | Cu   | 0.578  | -0.309 | 0.885 |
| Cu   | 10.833 | 5.668 | 6.644  | Cu   | 4.778  | 5.981  | 3.761 | Cu   | 2.436  | 3.778  | 0.908 |

**Table S38:** Coordinates for the most stable L-alanine adsorbed on Pt-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.137  | 3.927 | 9.895  | Cu   | 7.297  | 8.248  | 6.793 | Cu   | 3.092  | 2.032  | 3.781 |
| C    | 7.685  | 2.631 | 9.187  | Cu   | 5.395  | 4.213  | 6.714 | Cu   | 8.511  | 6.109  | 3.194 |
| C    | 9.593  | 4.393 | 9.649  | Cu   | 10.866 | 8.245  | 6.180 | Cu   | 6.665  | 2.046  | 3.221 |
| H    | 9.970  | 4.916 | 10.544 | Cu   | 9.049  | 4.189  | 6.186 | Cu   | 2.983  | 4.557  | 3.214 |
| H    | 9.925  | 2.504 | 9.253  | Cu   | 5.317  | 6.729  | 6.208 | Cu   | 1.124  | 0.492  | 3.229 |
| H    | 9.572  | 5.106 | 8.803  | Cu   | 3.526  | 2.615  | 6.203 | Cu   | 2.831  | 7.014  | 2.567 |
| H    | 8.011  | 3.709 | 10.974 | Cu   | 8.923  | 6.722  | 5.603 | Cu   | 0.983  | 2.937  | 2.525 |
| H    | 7.312  | 5.824 | 10.136 | Cu   | 7.103  | 2.677  | 5.595 | Cu   | 8.386  | 8.577  | 2.580 |
| H    | 6.254  | 4.665 | 9.586  | Cu   | 3.404  | 5.170  | 5.611 | Cu   | 6.531  | 4.509  | 2.543 |
| N    | 7.213  | 5.026 | 9.501  | Cu   | 1.576  | 1.109  | 5.624 | Cu   | 11.999 | 8.585  | 1.987 |
| O    | 6.444  | 2.503 | 8.984  | Cu   | -0.410 | -0.472 | 5.014 | Cu   | 10.136 | 4.519  | 1.938 |
| O    | 12.278 | 9.874 | 8.910  | Cu   | 1.445  | 3.559  | 4.907 | Cu   | 6.471  | 7.028  | 1.960 |
| O    | -0.562 | 0.207 | 9.338  | Cu   | 5.145  | 1.090  | 5.011 | Cu   | 4.627  | 2.974  | 1.946 |
|      |        |       |        | Cu   | 6.981  | 5.158  | 4.920 | Cu   | 10.031 | 7.022  | 1.407 |
|      |        |       |        | Cu   | 12.416 | 9.220  | 4.416 | Cu   | 8.188  | 2.962  | 1.403 |
| Pt   | 7.357  | 5.707 | 7.372  | Cu   | 10.551 | 5.137  | 4.352 | Cu   | 4.521  | 5.477  | 1.409 |
| Cu   | 5.582  | 1.696 | 7.338  | Cu   | 6.872  | 7.659  | 4.384 | Cu   | 2.679  | 1.403  | 1.416 |
| Cu   | 1.846  | 4.132 | 7.196  | Cu   | 5.027  | 3.595  | 4.369 | Cu   | 6.259  | 1.392  | 0.935 |
| Cu   | 0.075  | 0.203 | 7.326  | Cu   | 10.454 | 7.645  | 3.786 | Cu   | 8.082  | 5.446  | 0.902 |
| Cu   | 12.809 | 9.784 | 6.801  | Cu   | 8.617  | 3.589  | 3.781 | Cu   | 0.723  | -0.162 | 0.946 |
| Cu   | 10.971 | 5.781 | 6.688  | Cu   | 4.921  | 6.106  | 3.791 | Cu   | 2.576  | 3.917  | 0.939 |

**Table S39:** Coordinates for the most stable D- $\mu_3$ -serine adsorbed on Pt-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.543  | 4.559  | 9.996  | Cu   | 7.237  | 8.197  | 6.784 | Cu   | 3.015  | 1.939  | 3.820 |
| C    | 9.906  | 4.536  | 9.299  | Cu   | 5.346  | 4.131  | 6.773 | Cu   | 8.466  | 6.006  | 3.217 |
| C    | 7.760  | 3.268  | 9.682  | Cu   | 10.808 | 8.204  | 6.224 | Cu   | 6.615  | 1.966  | 3.255 |
| H    | 5.932  | 3.751  | 9.200  | Cu   | 8.990  | 4.116  | 6.210 | Cu   | 2.908  | 4.445  | 3.253 |
| H    | 8.182  | 2.440  | 10.266 | Cu   | 5.289  | 6.628  | 6.149 | Cu   | 1.067  | 0.393  | 3.241 |
| H    | 7.881  | 3.039  | 8.604  | Cu   | 3.420  | 2.570  | 6.232 | Cu   | 2.784  | 6.907  | 2.579 |
| H    | 8.681  | 4.646  | 11.089 | Cu   | 8.910  | 6.644  | 5.619 | Cu   | 0.924  | 2.846  | 2.578 |
| H    | 6.920  | 5.826  | 10.052 | Cu   | 7.049  | 2.603  | 5.640 | Cu   | 8.319  | 8.467  | 2.572 |
| H    | 8.355  | 6.579  | 9.629  | Cu   | 3.365  | 5.102  | 5.616 | Cu   | 6.487  | 4.409  | 2.549 |
| N    | 7.782  | 5.737  | 9.502  | Cu   | 1.491  | 1.021  | 5.663 | Cu   | 11.947 | 8.480  | 1.985 |
| O    | 10.341 | 5.638  | 8.836  | Cu   | -0.451 | -0.549 | 4.999 | Cu   | 10.100 | 4.429  | 1.997 |
| O    | -0.628 | 0.269  | 9.164  | Cu   | 1.355  | 3.468  | 4.994 | Cu   | 6.410  | 6.911  | 1.955 |
| O    | 6.376  | 3.392  | 10.004 | Cu   | 5.069  | 0.990  | 4.980 | Cu   | 4.563  | 2.868  | 1.982 |
|      |        |        |        | Cu   | 6.922  | 5.058  | 4.939 | Cu   | 9.990  | 6.920  | 1.425 |
|      |        |        |        | Cu   | 12.351 | 9.118  | 4.392 | Cu   | 8.157  | 2.872  | 1.439 |
| Pt   | 7.283  | 5.675  | 7.372  | Cu   | 10.517 | 5.074  | 4.458 | Cu   | 4.455  | 5.359  | 1.423 |
| Cu   | 5.476  | 1.675  | 7.270  | Cu   | 6.822  | 7.563  | 4.381 | Cu   | 2.602  | 1.299  | 1.448 |
| Cu   | 1.830  | 4.191  | 7.252  | Cu   | 4.971  | 3.506  | 4.393 | Cu   | 6.214  | 1.306  | 0.972 |
| Cu   | 0.015  | -0.095 | 7.345  | Cu   | 10.403 | 7.559  | 3.804 | Cu   | 8.058  | 5.348  | 0.917 |
| Cu   | 12.751 | 9.746  | 6.739  | Cu   | 8.577  | 3.503  | 3.816 | Cu   | 0.659  | -0.262 | 0.949 |
| Cu   | 10.964 | 5.717  | 6.892  | Cu   | 4.869  | 5.998  | 3.776 | Cu   | 2.511  | 3.789  | 0.969 |

**Table S40:** Coordinates for the most stable L- $\mu_3$ -serine adsorbed on Pt-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.438  | 5.023  | 9.811  | Cu   | 7.456  | 8.075 | 6.712 | Cu   | 3.195  | 1.829 | 3.777 |
| C    | 4.162  | 5.527  | 9.092  | Cu   | 5.519  | 4.032 | 6.710 | Cu   | 8.641  | 5.914 | 3.181 |
| C    | 5.694  | 3.517  | 9.701  | Cu   | 11.007 | 8.043 | 6.213 | Cu   | 6.774  | 1.853 | 3.164 |
| H    | 4.792  | 3.020  | 10.107 | Cu   | 9.175  | 4.036 | 6.203 | Cu   | 3.070  | 4.326 | 3.169 |
| H    | 6.546  | 3.271  | 10.370 | Cu   | 5.464  | 6.518 | 6.094 | Cu   | 1.247  | 0.287 | 3.201 |
| H    | 5.259  | 5.227  | 10.887 | Cu   | 3.611  | 2.420 | 6.150 | Cu   | 2.957  | 6.792 | 2.524 |
| H    | 7.363  | 5.752  | 10.062 | Cu   | 9.089  | 6.513 | 5.585 | Cu   | 1.121  | 2.755 | 2.571 |
| H    | 6.296  | 6.828  | 9.376  | Cu   | 7.228  | 2.470 | 5.520 | Cu   | 8.500  | 8.375 | 2.532 |
| N    | 6.608  | 5.848  | 9.375  | Cu   | 3.542  | 4.985 | 5.513 | Cu   | 6.647  | 4.300 | 2.497 |
| O    | 4.127  | 6.786  | 8.882  | Cu   | 1.674  | 0.888 | 5.632 | Cu   | 12.115 | 8.382 | 1.919 |
| O    | 3.254  | 4.677  | 8.847  | Cu   | 3.406  | 7.457 | 4.936 | Cu   | 10.291 | 4.320 | 1.937 |
| O    | 5.992  | 3.082  | 8.403  | Cu   | 1.572  | 3.396 | 5.013 | Cu   | 6.589  | 6.808 | 1.906 |
|      |        |        |        | Cu   | 8.978  | 8.998 | 4.959 | Cu   | 4.711  | 2.763 | 1.921 |
|      |        |        |        | Cu   | 7.121  | 4.933 | 4.905 | Cu   | 10.177 | 6.823 | 1.395 |
|      |        |        |        | Cu   | 12.522 | 8.997 | 4.333 | Cu   | 8.334  | 2.760 | 1.369 |
| Pt   | 7.501  | 5.605  | 7.359  | Cu   | 10.697 | 4.956 | 4.364 | Cu   | 4.608  | 5.245 | 1.363 |
| Cu   | 5.701  | 1.505  | 7.290  | Cu   | 7.003  | 7.458 | 4.324 | Cu   | 2.767  | 1.199 | 1.397 |
| Cu   | 2.086  | 4.122  | 7.321  | Cu   | 5.152  | 3.401 | 4.346 | Cu   | 10.057 | 9.318 | 0.891 |
| Cu   | 0.085  | -0.165 | 7.308  | Cu   | 10.590 | 7.452 | 3.770 | Cu   | 8.236  | 5.236 | 0.895 |
| Cu   | 12.889 | 9.656  | 6.663  | Cu   | 8.752  | 3.395 | 3.745 | Cu   | 4.529  | 7.728 | 0.907 |
| Cu   | 11.141 | 5.548  | 6.763  | Cu   | 5.054  | 5.888 | 3.727 | Cu   | 2.659  | 3.679 | 0.880 |

**Table S41:** Coordinates for the most stable D- $\mu_4$ -serine adsorbed on Pt-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 9.408  | 6.091  | 9.799  | Cu   | 7.092  | 8.004 | 6.695 | Cu   | 2.902  | 1.739 | 3.796 |
| C    | 10.164 | 7.276  | 9.154  | Cu   | 5.313  | 3.886 | 6.774 | Cu   | 8.333  | 5.788 | 3.169 |
| C    | 10.068 | 4.726  | 9.596  | Cu   | 10.716 | 7.991 | 6.045 | Cu   | 6.483  | 1.754 | 3.200 |
| H    | 11.049 | 4.772  | 10.107 | Cu   | 8.815  | 3.890 | 6.162 | Cu   | 2.800  | 4.252 | 3.226 |
| H    | 9.447  | 3.965  | 10.110 | Cu   | 5.149  | 6.385 | 6.187 | Cu   | 0.948  | 0.182 | 3.183 |
| H    | 9.454  | 6.286  | 10.890 | Cu   | 3.325  | 2.384 | 6.275 | Cu   | 2.670  | 6.702 | 2.502 |
| H    | 7.427  | 5.564  | 10.060 | Cu   | 8.796  | 6.461 | 5.536 | Cu   | 0.821  | 2.645 | 2.541 |
| H    | 7.665  | 7.093  | 9.456  | Cu   | 6.904  | 2.375 | 5.579 | Cu   | 8.206  | 8.261 | 2.554 |
| N    | 7.972  | 6.114  | 9.388  | Cu   | 3.209  | 4.851 | 5.683 | Cu   | 6.367  | 4.207 | 2.551 |
| O    | 9.461  | 8.313  | 8.923  | Cu   | 1.387  | 0.804 | 5.582 | Cu   | 11.822 | 8.273 | 1.922 |
| O    | 11.417 | 7.139  | 8.976  | Cu   | 3.127  | 7.331 | 4.939 | Cu   | 9.978  | 4.220 | 1.923 |
| O    | 10.227 | 4.371  | 8.246  | Cu   | 1.282  | 3.277 | 4.989 | Cu   | 6.293  | 6.708 | 1.925 |
|      |        |        |        | Cu   | 8.635  | 8.939 | 4.964 | Cu   | 4.447  | 2.667 | 1.968 |
|      |        |        |        | Cu   | 6.800  | 4.859 | 4.945 | Cu   | 9.860  | 6.707 | 1.371 |
|      |        |        |        | Cu   | 12.249 | 8.919 | 4.312 | Cu   | 8.011  | 2.667 | 1.397 |
| Pt   | 7.245  | 5.535  | 7.362  | Cu   | 10.398 | 4.852 | 4.363 | Cu   | 4.353  | 5.158 | 1.398 |
| Cu   | 5.447  | 1.351  | 7.325  | Cu   | 6.690  | 7.347 | 4.336 | Cu   | 2.509  | 1.099 | 1.412 |
| Cu   | 1.578  | 4.006  | 7.370  | Cu   | 4.836  | 3.311 | 4.388 | Cu   | 9.758  | 9.204 | 0.916 |
| Cu   | -0.136 | -0.286 | 7.280  | Cu   | 10.291 | 7.337 | 3.727 | Cu   | 7.912  | 5.135 | 0.871 |
| Cu   | 12.619 | 9.543  | 6.665  | Cu   | 8.460  | 3.295 | 3.774 | Cu   | 4.259  | 7.659 | 0.894 |
| Cu   | 10.815 | 5.500  | 6.713  | Cu   | 4.742  | 5.785 | 3.776 | Cu   | 2.404  | 3.592 | 0.937 |

**Table S42:** Coordinates for the most stable L- $\mu_4$ -serine adsorbed on Pt-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.441  | 4.358  | 9.953  | Cu   | 7.265  | 8.252  | 6.827 | Cu   | 3.035  | 1.982  | 3.858 |
| C    | 9.872  | 4.461  | 9.356  | Cu   | 5.352  | 4.206  | 6.728 | Cu   | 8.493  | 6.048  | 3.244 |
| C    | 7.815  | 3.071  | 9.393  | Cu   | 10.821 | 8.247  | 6.278 | Cu   | 6.626  | 1.999  | 3.269 |
| H    | 5.665  | 3.978  | 8.914  | Cu   | 9.011  | 4.155  | 6.214 | Cu   | 2.917  | 4.480  | 3.271 |
| H    | 8.299  | 2.198  | 9.848  | Cu   | 5.307  | 6.687  | 6.163 | Cu   | 1.095  | 0.436  | 3.282 |
| H    | 7.996  | 3.042  | 8.301  | Cu   | 3.458  | 2.611  | 6.262 | Cu   | 2.801  | 6.937  | 2.601 |
| H    | 8.501  | 4.308  | 11.056 | Cu   | 8.932  | 6.697  | 5.643 | Cu   | 0.938  | 2.885  | 2.612 |
| H    | 6.843  | 5.687  | 10.089 | Cu   | 7.060  | 2.639  | 5.656 | Cu   | 8.348  | 8.524  | 2.641 |
| H    | 8.312  | 6.386  | 9.705  | Cu   | 3.371  | 5.141  | 5.624 | Cu   | 6.505  | 4.440  | 2.562 |
| N    | 7.700  | 5.576  | 9.539  | Cu   | 1.503  | 1.079  | 5.717 | Cu   | 11.955 | 8.515  | 2.004 |
| O    | 10.259 | 5.600  | 8.957  | Cu   | -0.434 | -0.509 | 5.015 | Cu   | 10.126 | 4.460  | 2.027 |
| O    | -0.579 | 0.235  | 9.234  | Cu   | 1.363  | 3.507  | 5.028 | Cu   | 6.448  | 6.948  | 1.988 |
| S    | 6.016  | 2.823  | 9.589  | Cu   | 5.112  | 1.070  | 5.087 | Cu   | 4.576  | 2.906  | 1.997 |
|      |        |        |        | Cu   | 6.948  | 5.104  | 4.942 | Cu   | 9.999  | 6.959  | 1.459 |
|      |        |        |        | Cu   | 12.357 | 9.153  | 4.407 | Cu   | 8.173  | 2.898  | 1.452 |
| Pt   | 7.303  | 5.721  | 7.371  | Cu   | 10.535 | 5.114  | 4.488 | Cu   | 4.474  | 5.390  | 1.444 |
| Cu   | 5.534  | 1.748  | 7.443  | Cu   | 6.853  | 7.617  | 4.419 | Cu   | 2.629  | 1.333  | 1.483 |
| Cu   | 1.844  | 4.212  | 7.277  | Cu   | 4.987  | 3.541  | 4.398 | Cu   | 6.212  | 1.334  | 0.987 |
| Cu   | 0.021  | -0.066 | 7.372  | Cu   | 10.417 | 7.607  | 3.841 | Cu   | 8.086  | 5.371  | 0.946 |
| Cu   | 12.778 | 9.768  | 6.740  | Cu   | 8.592  | 3.534  | 3.827 | Cu   | 0.690  | -0.231 | 0.991 |
| Cu   | 10.940 | 5.760  | 6.957  | Cu   | 4.890  | 6.036  | 3.793 | Cu   | 2.523  | 3.818  | 0.995 |

**Table S43:** Coordinates for the most stable D- $\mu_3$ -cysteine adsorbed on Pt-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.441  | 4.358  | 9.953  | Cu   | 7.265  | 8.252  | 6.827 | Cu   | 3.035  | 1.982  | 3.858 |
| C    | 9.872  | 4.461  | 9.356  | Cu   | 5.352  | 4.206  | 6.728 | Cu   | 8.493  | 6.048  | 3.244 |
| C    | 7.815  | 3.071  | 9.393  | Cu   | 10.821 | 8.247  | 6.278 | Cu   | 6.626  | 1.999  | 3.269 |
| H    | 5.665  | 3.978  | 8.914  | Cu   | 9.011  | 4.155  | 6.214 | Cu   | 2.917  | 4.480  | 3.271 |
| H    | 8.299  | 2.198  | 9.848  | Cu   | 5.307  | 6.687  | 6.163 | Cu   | 1.095  | 0.436  | 3.282 |
| H    | 7.996  | 3.042  | 8.301  | Cu   | 3.458  | 2.611  | 6.262 | Cu   | 2.801  | 6.937  | 2.601 |
| H    | 8.501  | 4.308  | 11.056 | Cu   | 8.932  | 6.697  | 5.643 | Cu   | 0.938  | 2.885  | 2.612 |
| H    | 6.843  | 5.687  | 10.089 | Cu   | 7.060  | 2.639  | 5.656 | Cu   | 8.348  | 8.524  | 2.641 |
| H    | 8.312  | 6.386  | 9.705  | Cu   | 3.371  | 5.141  | 5.624 | Cu   | 6.505  | 4.440  | 2.562 |
| N    | 7.700  | 5.576  | 9.539  | Cu   | 1.503  | 1.079  | 5.717 | Cu   | 11.955 | 8.515  | 2.004 |
| O    | 10.259 | 5.600  | 8.957  | Cu   | -0.434 | -0.509 | 5.015 | Cu   | 10.126 | 4.460  | 2.027 |
| O    | -0.579 | 0.235  | 9.234  | Cu   | 1.363  | 3.507  | 5.028 | Cu   | 6.448  | 6.948  | 1.988 |
| S    | 6.016  | 2.823  | 9.589  | Cu   | 5.112  | 1.070  | 5.087 | Cu   | 4.576  | 2.906  | 1.997 |
|      |        |        |        | Cu   | 6.948  | 5.104  | 4.942 | Cu   | 9.999  | 6.959  | 1.459 |
|      |        |        |        | Cu   | 12.357 | 9.153  | 4.407 | Cu   | 8.173  | 2.898  | 1.452 |
| Pt   | 7.303  | 5.721  | 7.371  | Cu   | 10.535 | 5.114  | 4.488 | Cu   | 4.474  | 5.390  | 1.444 |
| Cu   | 5.534  | 1.748  | 7.443  | Cu   | 6.853  | 7.617  | 4.419 | Cu   | 2.629  | 1.333  | 1.483 |
| Cu   | 1.844  | 4.212  | 7.277  | Cu   | 4.987  | 3.541  | 4.398 | Cu   | 6.212  | 1.334  | 0.987 |
| Cu   | 0.021  | -0.066 | 7.372  | Cu   | 10.417 | 7.607  | 3.841 | Cu   | 8.086  | 5.371  | 0.946 |
| Cu   | 12.778 | 9.768  | 6.740  | Cu   | 8.592  | 3.534  | 3.827 | Cu   | 0.690  | -0.231 | 0.991 |
| Cu   | 10.940 | 5.760  | 6.957  | Cu   | 4.890  | 6.036  | 3.793 | Cu   | 2.523  | 3.818  | 0.995 |

**Table S44:** Coordinates for the most stable L- $\mu_3$ -cysteine adsorbed on Pt-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.426  | 5.312  | 9.903  | Cu   | 7.468  | 7.967 | 6.723 | Cu   | 3.180  | 1.761 | 3.754 |
| C    | 4.123  | 5.604  | 9.115  | Cu   | 5.413  | 3.943 | 6.671 | Cu   | 8.627  | 5.851 | 3.190 |
| C    | 5.842  | 3.848  | 9.957  | Cu   | 11.011 | 7.979 | 6.201 | Cu   | 6.749  | 1.783 | 3.119 |
| H    | 4.947  | 3.230  | 10.098 | Cu   | 9.135  | 3.987 | 6.164 | Cu   | 3.052  | 4.261 | 3.137 |
| H    | 6.532  | 3.683  | 10.800 | Cu   | 5.438  | 6.467 | 6.081 | Cu   | 1.241  | 0.226 | 3.176 |
| H    | 5.197  | 5.626  | 10.941 | Cu   | 3.587  | 2.321 | 6.142 | Cu   | 2.942  | 6.721 | 2.487 |
| H    | 7.271  | 6.266  | 10.066 | Cu   | 9.062  | 6.445 | 5.625 | Cu   | 1.108  | 2.697 | 2.557 |
| H    | 6.121  | 7.119  | 9.217  | Cu   | 7.220  | 2.396 | 5.439 | Cu   | 8.481  | 8.310 | 2.521 |
| N    | 6.517  | 6.184  | 9.377  | Cu   | 3.518  | 4.935 | 5.465 | Cu   | 6.639  | 4.238 | 2.498 |
| O    | 3.926  | 6.842  | 8.882  | Cu   | 1.667  | 0.821 | 5.604 | Cu   | 12.088 | 8.318 | 1.895 |
| O    | 3.357  | 4.632  | 8.844  | Cu   | 3.384  | 7.403 | 4.897 | Cu   | 10.283 | 4.256 | 1.919 |
| S    | 6.726  | 3.257  | 8.450  | Cu   | 1.574  | 3.341 | 4.999 | Cu   | 6.579  | 6.753 | 1.904 |
|      |        |        |        | Cu   | 8.963  | 8.935 | 4.946 | Cu   | 4.701  | 2.700 | 1.883 |
|      |        |        |        | Cu   | 7.094  | 4.871 | 4.913 | Cu   | 10.160 | 6.757 | 1.391 |
|      |        |        |        | Cu   | 12.503 | 8.938 | 4.293 | Cu   | 8.310  | 2.698 | 1.341 |
| Pt   | 7.402  | 5.473  | 7.418  | Cu   | 10.686 | 4.898 | 4.354 | Cu   | 4.614  | 5.181 | 1.348 |
| Cu   | 5.729  | 1.520  | 7.249  | Cu   | 6.997  | 7.391 | 4.331 | Cu   | 2.760  | 1.144 | 1.372 |
| Cu   | 2.133  | 4.075  | 7.313  | Cu   | 5.116  | 3.329 | 4.304 | Cu   | 10.029 | 9.238 | 0.857 |
| Cu   | 0.053  | -0.177 | 7.249  | Cu   | 10.563 | 7.384 | 3.773 | Cu   | 8.225  | 5.182 | 0.894 |
| Cu   | 12.876 | 9.593  | 6.623  | Cu   | 8.740  | 3.340 | 3.709 | Cu   | 4.523  | 7.667 | 0.887 |
| Cu   | 11.147 | 5.497  | 6.736  | Cu   | 5.044  | 5.834 | 3.710 | Cu   | 2.645  | 3.625 | 0.854 |

**Table S45:** Coordinates for the most stable D- $\mu_4$ -cysteine adsorbed on Pt-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.337  | 4.351  | 9.874  | Cu   | 7.276  | 8.282  | 6.791 | Cu   | 3.064  | 1.978  | 3.885 |
| C    | 9.780  | 4.423  | 9.316  | Cu   | 5.411  | 4.181  | 7.024 | Cu   | 8.513  | 6.041  | 3.256 |
| C    | 7.644  | 3.099  | 9.274  | Cu   | 10.863 | 8.238  | 6.259 | Cu   | 6.654  | 2.007  | 3.286 |
| H    | 7.915  | 2.225  | 9.881  | Cu   | 9.039  | 4.156  | 6.214 | Cu   | 2.952  | 4.477  | 3.316 |
| H    | 8.049  | 2.940  | 8.256  | Cu   | 5.341  | 6.657  | 6.187 | Cu   | 1.122  | 0.433  | 3.293 |
| H    | 8.378  | 4.253  | 10.974 | Cu   | 3.473  | 2.617  | 6.271 | Cu   | 2.838  | 6.938  | 2.622 |
| H    | 6.713  | 5.631  | 9.955  | Cu   | 8.980  | 6.714  | 5.616 | Cu   | 0.981  | 2.888  | 2.637 |
| H    | 8.198  | 6.408  | 9.832  | Cu   | 7.089  | 2.632  | 5.665 | Cu   | 8.374  | 8.509  | 2.628 |
| N    | 7.639  | 5.608  | 9.513  | Cu   | 3.444  | 5.123  | 5.695 | Cu   | 6.524  | 4.435  | 2.590 |
| O    | 10.207 | 5.553  | 8.918  | Cu   | 1.511  | 1.068  | 5.740 | Cu   | 11.997 | 8.521  | 2.014 |
| O    | -0.682 | 0.188  | 9.217  | Cu   | -0.395 | -0.518 | 5.042 | Cu   | 10.156 | 4.463  | 2.044 |
| S    | 5.815  | 3.131  | 9.081  | Cu   | 1.390  | 3.504  | 5.063 | Cu   | 6.465  | 6.944  | 1.998 |
|      |        |        |        | Cu   | 5.138  | 1.060  | 5.049 | Cu   | 4.601  | 2.903  | 2.060 |
|      |        |        |        | Cu   | 6.966  | 5.086  | 4.979 | Cu   | 10.035 | 6.961  | 1.467 |
|      |        |        |        | Cu   | 12.403 | 9.153  | 4.427 | Cu   | 8.208  | 2.903  | 1.471 |
| Pt   | 7.410  | 5.820  | 7.354  | Cu   | 10.569 | 5.113  | 4.496 | Cu   | 4.497  | 5.389  | 1.466 |
| Cu   | 5.536  | 1.655  | 7.401  | Cu   | 6.871  | 7.602  | 4.414 | Cu   | 2.657  | 1.335  | 1.501 |
| Cu   | 1.864  | 4.212  | 7.311  | Cu   | 5.034  | 3.567  | 4.507 | Cu   | 6.245  | 1.351  | 1.001 |
| Cu   | 0.060  | -0.100 | 7.412  | Cu   | 10.462 | 7.609  | 3.829 | Cu   | 8.104  | 5.367  | 0.965 |
| Cu   | 12.809 | 9.764  | 6.762  | Cu   | 8.623  | 3.529  | 3.846 | Cu   | 0.711  | -0.232 | 0.995 |
| Cu   | 10.959 | 5.750  | 6.988  | Cu   | 4.918  | 6.029  | 3.816 | Cu   | 2.567  | 3.817  | 1.023 |

**Table S46:** Coordinates for the most stable L- $\mu_4$ -cysteine adsorbed on Pt-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 7.957  | 4.061 | 9.970  | Cu   | 7.346  | 8.220  | 6.744 | Cu   | 3.113  | 1.962  | 3.750 |
| C    | 7.707  | 2.795 | 9.126  | Cu   | 5.438  | 4.180  | 6.660 | Cu   | 8.531  | 6.034  | 3.146 |
| C    | 9.402  | 4.523 | 9.962  | Cu   | 10.848 | 8.181  | 6.156 | Cu   | 6.668  | 1.970  | 3.160 |
| H    | 9.535  | 5.421 | 10.586 | Cu   | 9.029  | 4.135  | 6.131 | Cu   | 2.984  | 4.484  | 3.169 |
| H    | 10.058 | 3.725 | 10.335 | Cu   | 5.325  | 6.689  | 6.173 | Cu   | 1.139  | 0.422  | 3.200 |
| H    | 9.702  | 4.771 | 8.926  | Cu   | 3.583  | 2.558  | 6.173 | Cu   | 2.832  | 6.929  | 2.502 |
| H    | 7.637  | 3.826 | 11.003 | Cu   | 8.937  | 6.661  | 5.537 | Cu   | 0.998  | 2.866  | 2.489 |
| H    | 7.140  | 5.970 | 10.030 | Cu   | 7.117  | 2.613  | 5.526 | Cu   | 8.399  | 8.501  | 2.535 |
| H    | 6.097  | 4.801 | 9.475  | Cu   | 3.423  | 5.125  | 5.563 | Cu   | 6.546  | 4.438  | 2.493 |
| N    | 7.067  | 5.137 | 9.435  | Cu   | 1.604  | 1.053  | 5.594 | Cu   | 12.004 | 8.506  | 1.934 |
| O    | 6.477  | 2.508 | 8.925  | Cu   | -0.434 | -0.561 | 4.919 | Cu   | 10.157 | 4.444  | 1.898 |
| O    | 8.720  | 2.161 | 8.709  | Cu   | 1.441  | 3.482  | 4.848 | Cu   | 6.486  | 6.946  | 1.924 |
|      |        |       |        | Cu   | 5.170  | 1.038  | 4.973 | Cu   | 4.633  | 2.896  | 1.897 |
|      |        |       |        | Cu   | 6.997  | 5.102  | 4.874 | Cu   | 10.052 | 6.947  | 1.360 |
|      |        |       |        | Cu   | 12.409 | 9.148  | 4.375 | Cu   | 8.196  | 2.886  | 1.349 |
| Pt   | 7.387  | 5.705 | 7.326  | Cu   | 10.566 | 5.066  | 4.325 | Cu   | 4.528  | 5.393  | 1.371 |
| Pt   | 1.841  | 4.038 | 7.237  | Cu   | 6.886  | 7.596  | 4.345 | Cu   | 2.690  | 1.330  | 1.379 |
| Cu   | 5.649  | 1.684 | 7.317  | Cu   | 5.042  | 3.535  | 4.318 | Cu   | 6.262  | 1.311  | 0.876 |
| Cu   | 0.012  | 0.135 | 7.184  | Cu   | 10.466 | 7.580  | 3.746 | Cu   | 8.102  | 5.371  | 0.856 |
| Cu   | 12.804 | 9.729 | 6.801  | Cu   | 8.624  | 3.517  | 3.723 | Cu   | 0.744  | -0.240 | 0.916 |
| Cu   | 10.927 | 5.693 | 6.709  | Cu   | 4.932  | 6.035  | 3.753 | Cu   | 2.578  | 3.834  | 0.885 |

**Table S47:** Coordinates for the most stable D-alanine adsorbed on Pt-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 7.341  | 4.116 | 10.048 | Cu   | 7.097  | 8.260  | 6.773 | Cu   | 2.882  | 2.018  | 3.784 |
| C    | 7.307  | 2.838 | 9.184  | Cu   | 5.217  | 4.218  | 6.749 | Cu   | 8.299  | 6.083  | 3.195 |
| C    | 5.970  | 4.659 | 10.408 | Cu   | 10.637 | 8.243  | 6.184 | Cu   | 6.437  | 2.028  | 3.207 |
| H    | 6.067  | 5.569 | 11.021 | Cu   | 8.834  | 4.188  | 6.147 | Cu   | 2.760  | 4.545  | 3.219 |
| H    | 5.395  | 3.908 | 10.965 | Cu   | 5.136  | 6.713  | 6.206 | Cu   | 0.912  | 0.472  | 3.228 |
| H    | 5.419  | 4.911 | 9.487  | Cu   | 3.341  | 2.611  | 6.217 | Cu   | 2.600  | 6.986  | 2.540 |
| H    | 7.914  | 3.872 | 10.962 | Cu   | 8.751  | 6.730  | 5.569 | Cu   | 0.771  | 2.922  | 2.528 |
| H    | 8.284  | 5.962 | 9.851  | Cu   | 6.882  | 2.668  | 5.580 | Cu   | 8.165  | 8.551  | 2.568 |
| H    | 9.013  | 4.740 | 8.988  | Cu   | 3.200  | 5.195  | 5.626 | Cu   | 6.311  | 4.496  | 2.544 |
| N    | 8.103  | 5.138 | 9.268  | Cu   | 1.383  | 1.100  | 5.610 | Cu   | 11.773 | 8.563  | 1.976 |
| O    | 8.432  | 2.469 | 8.716  | Cu   | -0.652 | -0.505 | 4.960 | Cu   | 9.924  | 4.495  | 1.933 |
| O    | 6.179  | 2.281 | 9.003  | Cu   | 1.224  | 3.545  | 4.893 | Cu   | 6.256  | 7.000  | 1.955 |
|      |        |       |        | Cu   | 4.930  | 1.087  | 4.994 | Cu   | 4.404  | 2.953  | 1.947 |
|      |        |       |        | Cu   | 6.752  | 5.148  | 4.924 | Cu   | 9.819  | 6.997  | 1.399 |
|      |        |       |        | Cu   | 12.188 | 9.217  | 4.423 | Cu   | 7.956  | 2.942  | 1.393 |
| Pt   | 7.197  | 5.752 | 7.355  | Cu   | 10.347 | 5.126  | 4.353 | Cu   | 4.298  | 5.448  | 1.409 |
| Pt   | 1.617  | 4.118 | 7.290  | Cu   | 6.661  | 7.641  | 4.376 | Cu   | 2.463  | 1.386  | 1.409 |
| Cu   | 5.375  | 1.676 | 7.329  | Cu   | 4.805  | 3.591  | 4.380 | Cu   | 6.026  | 1.362  | 0.921 |
| Cu   | -0.167 | 0.175 | 7.220  | Cu   | 10.246 | 7.640  | 3.778 | Cu   | 7.866  | 5.422  | 0.899 |
| Cu   | 12.567 | 9.813 | 6.882  | Cu   | 8.391  | 3.575  | 3.768 | Cu   | 0.513  | -0.186 | 0.950 |
| Cu   | 10.736 | 5.735 | 6.745  | Cu   | 4.697  | 6.091  | 3.789 | Cu   | 2.350  | 3.893  | 0.934 |

**Table S48:** Coordinates for the most stable L-alanine adsorbed on Pt-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.127  | 3.958 | 9.904  | Cu   | 7.308  | 8.240  | 6.792 | Cu   | 3.104  | 2.021  | 3.774 |
| C    | 7.669  | 2.654 | 9.214  | Cu   | 5.399  | 4.207  | 6.716 | Cu   | 8.510  | 6.103  | 3.192 |
| C    | 9.591  | 4.405 | 9.652  | Cu   | 10.848 | 8.241  | 6.186 | Cu   | 6.663  | 2.041  | 3.217 |
| H    | 9.977  | 4.923 | 10.546 | Cu   | 9.052  | 4.171  | 6.191 | Cu   | 2.984  | 4.553  | 3.197 |
| H    | 9.895  | 2.507 | 9.270  | Cu   | 5.321  | 6.727  | 6.210 | Cu   | 1.130  | 0.495  | 3.228 |
| H    | 9.577  | 5.120 | 8.808  | Cu   | 3.555  | 2.583  | 6.202 | Cu   | 2.833  | 7.016  | 2.570 |
| H    | 7.997  | 3.759 | 10.986 | Cu   | 8.922  | 6.707  | 5.592 | Cu   | 0.988  | 2.935  | 2.512 |
| H    | 7.307  | 5.862 | 10.116 | Cu   | 7.111  | 2.664  | 5.600 | Cu   | 8.387  | 8.571  | 2.573 |
| H    | 6.248  | 4.700 | 9.579  | Cu   | 3.425  | 5.180  | 5.582 | Cu   | 6.532  | 4.509  | 2.541 |
| N    | 7.209  | 5.055 | 9.492  | Cu   | 1.576  | 1.093  | 5.623 | Cu   | 12.003 | 8.577  | 1.975 |
| O    | 6.428  | 2.535 | 8.993  | Cu   | -0.408 | -0.471 | 5.017 | Cu   | 10.134 | 4.520  | 1.939 |
| O    | 12.256 | 9.889 | 8.966  | Cu   | 1.445  | 3.543  | 4.867 | Cu   | 6.469  | 7.028  | 1.959 |
| O    | -0.579 | 0.209 | 9.335  | Cu   | 5.154  | 1.082  | 5.012 | Cu   | 4.629  | 2.974  | 1.933 |
|      |        |       |        | Cu   | 6.977  | 5.151  | 4.919 | Cu   | 10.033 | 7.018  | 1.401 |
|      |        |       |        | Cu   | 12.413 | 9.220  | 4.404 | Cu   | 8.191  | 2.961  | 1.406 |
| Pt   | 7.361  | 5.707 | 7.365  | Cu   | 10.555 | 5.132  | 4.352 | Cu   | 4.520  | 5.476  | 1.402 |
| Pt   | 1.853  | 4.097 | 7.260  | Cu   | 6.874  | 7.653  | 4.384 | Cu   | 2.684  | 1.406  | 1.400 |
| Cu   | 5.595  | 1.696 | 7.354  | Cu   | 5.034  | 3.585  | 4.363 | Cu   | 6.261  | 1.386  | 0.931 |
| Cu   | 0.080  | 0.192 | 7.341  | Cu   | 10.457 | 7.642  | 3.784 | Cu   | 8.081  | 5.445  | 0.898 |
| Cu   | 12.818 | 9.775 | 6.814  | Cu   | 8.616  | 3.585  | 3.785 | Cu   | 0.721  | -0.158 | 0.946 |
| Cu   | 10.945 | 5.757 | 6.704  | Cu   | 4.923  | 6.104  | 3.786 | Cu   | 2.576  | 3.906  | 0.916 |

**Table S49:** Coordinates for the most stable D- $\mu_3$ -serine adsorbed on Pt-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.533  | 4.549  | 10.002 | Cu   | 7.241  | 8.192  | 6.788 | Cu   | 3.024  | 1.938  | 3.820 |
| C    | 9.897  | 4.530  | 9.304  | Cu   | 5.345  | 4.131  | 6.777 | Cu   | 8.466  | 6.005  | 3.217 |
| C    | 7.755  | 3.258  | 9.677  | Cu   | 10.790 | 8.208  | 6.236 | Cu   | 6.611  | 1.967  | 3.253 |
| H    | 5.928  | 3.753  | 9.205  | Cu   | 8.995  | 4.119  | 6.211 | Cu   | 2.910  | 4.447  | 3.236 |
| H    | 8.180  | 2.426  | 10.253 | Cu   | 5.291  | 6.634  | 6.150 | Cu   | 1.070  | 0.395  | 3.237 |
| H    | 7.880  | 3.039  | 8.598  | Cu   | 3.439  | 2.548  | 6.235 | Cu   | 2.782  | 6.911  | 2.580 |
| H    | 8.669  | 4.632  | 11.096 | Cu   | 8.905  | 6.643  | 5.618 | Cu   | 0.929  | 2.849  | 2.577 |
| H    | 6.916  | 5.826  | 10.062 | Cu   | 7.051  | 2.604  | 5.641 | Cu   | 8.321  | 8.466  | 2.571 |
| H    | 8.355  | 6.567  | 9.635  | Cu   | 3.382  | 5.117  | 5.582 | Cu   | 6.489  | 4.411  | 2.548 |
| N    | 7.775  | 5.729  | 9.510  | Cu   | 1.495  | 1.018  | 5.652 | Cu   | 11.947 | 8.480  | 1.988 |
| O    | 10.324 | 5.633  | 8.842  | Cu   | -0.450 | -0.537 | 4.999 | Cu   | 10.100 | 4.428  | 1.991 |
| O    | -0.633 | 0.264  | 9.164  | Cu   | 1.358  | 3.474  | 4.963 | Cu   | 6.414  | 6.910  | 1.954 |
| O    | 6.370  | 3.371  | 9.998  | Cu   | 5.073  | 0.994  | 4.989 | Cu   | 4.559  | 2.870  | 1.977 |
|      |        |        |        | Cu   | 6.920  | 5.059  | 4.941 | Cu   | 9.992  | 6.919  | 1.428 |
|      |        |        |        | Cu   | 12.345 | 9.132  | 4.389 | Cu   | 8.156  | 2.872  | 1.433 |
| Pt   | 7.279  | 5.672  | 7.376  | Cu   | 10.520 | 5.078  | 4.446 | Cu   | 4.452  | 5.358  | 1.416 |
| Pt   | 1.848  | 4.198  | 7.328  | Cu   | 6.825  | 7.563  | 4.379 | Cu   | 2.604  | 1.300  | 1.445 |
| Cu   | 5.486  | 1.680  | 7.283  | Cu   | 4.974  | 3.506  | 4.391 | Cu   | 6.213  | 1.305  | 0.971 |
| Cu   | 0.036  | -0.074 | 7.350  | Cu   | 10.402 | 7.566  | 3.810 | Cu   | 8.060  | 5.350  | 0.913 |
| Cu   | 12.759 | 9.775  | 6.753  | Cu   | 8.575  | 3.505  | 3.815 | Cu   | 0.662  | -0.266 | 0.950 |
| Cu   | 10.943 | 5.702  | 6.885  | Cu   | 4.872  | 6.001  | 3.774 | Cu   | 2.501  | 3.787  | 0.953 |

**Table S50:** Coordinates for the most stable L- $\mu_3$ -serine adsorbed on Pt-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.489  | 5.033  | 9.838  | Cu   | 7.461  | 8.083 | 6.706 | Cu   | 3.192  | 1.829 | 3.771 |
| C    | 4.198  | 5.529  | 9.143  | Cu   | 5.527  | 4.055 | 6.716 | Cu   | 8.635  | 5.906 | 3.168 |
| C    | 5.729  | 3.523  | 9.711  | Cu   | 10.942 | 8.054 | 6.186 | Cu   | 6.765  | 1.849 | 3.159 |
| H    | 4.827  | 3.036  | 10.125 | Cu   | 9.175  | 4.022 | 6.204 | Cu   | 3.066  | 4.323 | 3.169 |
| H    | 6.591  | 3.260  | 10.359 | Cu   | 5.468  | 6.528 | 6.103 | Cu   | 1.242  | 0.284 | 3.199 |
| H    | 5.331  | 5.229  | 10.918 | Cu   | 3.596  | 2.429 | 6.160 | Cu   | 2.957  | 6.791 | 2.527 |
| H    | 7.411  | 5.778  | 10.062 | Cu   | 9.076  | 6.503 | 5.559 | Cu   | 1.114  | 2.746 | 2.533 |
| H    | 6.327  | 6.837  | 9.376  | Cu   | 7.225  | 2.471 | 5.513 | Cu   | 8.491  | 8.366 | 2.514 |
| N    | 6.648  | 5.859  | 9.382  | Cu   | 3.541  | 4.997 | 5.526 | Cu   | 6.645  | 4.297 | 2.504 |
| O    | 4.163  | 6.777  | 8.872  | Cu   | 1.666  | 0.887 | 5.626 | Cu   | 12.117 | 8.372 | 1.905 |
| O    | 3.285  | 4.665  | 8.984  | Cu   | 3.396  | 7.457 | 4.944 | Cu   | 10.280 | 4.319 | 1.925 |
| O    | 5.992  | 3.098  | 8.400  | Cu   | 1.530  | 3.382 | 4.936 | Cu   | 6.575  | 6.802 | 1.917 |
|      |        |        |        | Cu   | 8.957  | 9.012 | 4.950 | Cu   | 4.712  | 2.758 | 1.918 |
|      |        |        |        | Cu   | 7.120  | 4.937 | 4.908 | Cu   | 10.170 | 6.814 | 1.372 |
|      |        |        |        | Cu   | 12.514 | 9.005 | 4.319 | Cu   | 8.331  | 2.754 | 1.375 |
| Pt   | 7.518  | 5.619  | 7.358  | Cu   | 10.688 | 4.948 | 4.348 | Cu   | 4.608  | 5.244 | 1.370 |
| Pt   | 1.972  | 4.070  | 7.324  | Cu   | 6.997  | 7.460 | 4.321 | Cu   | 2.766  | 1.197 | 1.386 |
| Cu   | 5.699  | 1.528  | 7.287  | Cu   | 5.144  | 3.404 | 4.351 | Cu   | 10.060 | 9.311 | 0.883 |
| Cu   | 0.080  | -0.168 | 7.320  | Cu   | 10.572 | 7.456 | 3.746 | Cu   | 8.219  | 5.235 | 0.885 |
| Cu   | 12.872 | 9.654  | 6.681  | Cu   | 8.748  | 3.390 | 3.748 | Cu   | 4.523  | 7.733 | 0.905 |
| Cu   | 11.124 | 5.540  | 6.763  | Cu   | 5.044  | 5.882 | 3.743 | Cu   | 2.664  | 3.676 | 0.864 |

**Table S51:** Coordinates for the most stable D- $\mu_4$ -serine adsorbed on Pt-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 9.366  | 6.083  | 9.820  | Cu   | 7.099  | 8.004 | 6.696 | Cu   | 2.922  | 1.733 | 3.790 |
| C    | 10.123 | 7.288  | 9.217  | Cu   | 5.311  | 3.889 | 6.771 | Cu   | 8.332  | 5.780 | 3.167 |
| C    | 10.046 | 4.730  | 9.595  | Cu   | 10.713 | 7.989 | 6.071 | Cu   | 6.489  | 1.747 | 3.203 |
| H    | 11.035 | 4.795  | 10.086 | Cu   | 8.832  | 3.891 | 6.165 | Cu   | 2.808  | 4.251 | 3.194 |
| H    | 9.449  | 3.955  | 10.114 | Cu   | 5.156  | 6.398 | 6.182 | Cu   | 0.954  | 0.188 | 3.180 |
| H    | 9.396  | 6.249  | 10.917 | Cu   | 3.347  | 2.379 | 6.275 | Cu   | 2.672  | 6.703 | 2.503 |
| H    | 7.378  | 5.559  | 10.054 | Cu   | 8.792  | 6.455 | 5.529 | Cu   | 0.823  | 2.642 | 2.525 |
| H    | 7.633  | 7.087  | 9.450  | Cu   | 6.918  | 2.374 | 5.592 | Cu   | 8.213  | 8.257 | 2.552 |
| N    | 7.936  | 6.105  | 9.389  | Cu   | 3.252  | 4.861 | 5.607 | Cu   | 6.372  | 4.204 | 2.544 |
| O    | 9.403  | 8.299  | 8.916  | Cu   | 1.398  | 0.808 | 5.574 | Cu   | 11.826 | 8.265 | 1.919 |
| O    | 11.388 | 7.191  | 9.154  | Cu   | 3.132  | 7.341 | 4.938 | Cu   | 9.975  | 4.217 | 1.919 |
| O    | 10.187 | 4.380  | 8.239  | Cu   | 1.292  | 3.272 | 4.932 | Cu   | 6.301  | 6.707 | 1.921 |
|      |        |        |        | Cu   | 8.651  | 8.936 | 4.972 | Cu   | 4.452  | 2.664 | 1.958 |
|      |        |        |        | Cu   | 6.800  | 4.859 | 4.941 | Cu   | 9.857  | 6.705 | 1.373 |
|      |        |        |        | Cu   | 12.252 | 8.925 | 4.311 | Cu   | 8.014  | 2.661 | 1.396 |
| Pt   | 7.242  | 5.530  | 7.358  | Cu   | 10.404 | 4.852 | 4.358 | Cu   | 4.356  | 5.154 | 1.383 |
| Pt   | 1.661  | 3.989  | 7.372  | Cu   | 6.696  | 7.349 | 4.332 | Cu   | 2.514  | 1.097 | 1.403 |
| Cu   | 5.454  | 1.359  | 7.338  | Cu   | 4.854  | 3.303 | 4.374 | Cu   | 9.765  | 9.200 | 0.915 |
| Cu   | -0.105 | -0.247 | 7.277  | Cu   | 10.296 | 7.339 | 3.737 | Cu   | 7.913  | 5.129 | 0.864 |
| Cu   | 12.650 | 9.550  | 6.686  | Cu   | 8.459  | 3.293 | 3.778 | Cu   | 4.260  | 7.654 | 0.897 |
| Cu   | 10.812 | 5.517  | 6.717  | Cu   | 4.752  | 5.789 | 3.760 | Cu   | 2.403  | 3.581 | 0.911 |

**Table S52:** Coordinates for the most stable L- $\mu_4$ -serine adsorbed on Pt-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.050  | 4.063 | 9.919  | Cu   | 7.323  | 8.246  | 6.769 | Cu   | 3.117  | 1.989  | 3.761 |
| C    | 7.616  | 2.757 | 9.204  | Cu   | 5.413  | 4.206  | 6.696 | Cu   | 8.537  | 6.067  | 3.178 |
| C    | 9.475  | 4.613 | 9.702  | Cu   | 10.851 | 8.230  | 6.195 | Cu   | 6.683  | 2.008  | 3.205 |
| H    | 9.714  | 5.312 | 10.517 | Cu   | 9.062  | 4.162  | 6.190 | Cu   | 2.997  | 4.517  | 3.204 |
| H    | 9.918  | 2.352 | 9.433  | Cu   | 5.330  | 6.718  | 6.182 | Cu   | 1.141  | 0.446  | 3.211 |
| H    | 9.475  | 5.178 | 8.752  | Cu   | 3.557  | 2.584  | 6.185 | Cu   | 2.852  | 6.971  | 2.569 |
| H    | 7.912  | 3.853 | 10.998 | Cu   | 8.942  | 6.689  | 5.577 | Cu   | 1.006  | 2.892  | 2.520 |
| H    | 7.209  | 5.963 | 10.097 | Cu   | 7.125  | 2.650  | 5.586 | Cu   | 8.405  | 8.530  | 2.559 |
| H    | 6.155  | 4.784 | 9.568  | Cu   | 3.429  | 5.171  | 5.589 | Cu   | 6.554  | 4.465  | 2.525 |
| N    | 7.115  | 5.142 | 9.490  | Cu   | 1.592  | 1.074  | 5.594 | Cu   | 12.026 | 8.537  | 1.976 |
| O    | 6.374  | 2.644 | 8.966  | Cu   | -0.402 | -0.492 | 5.018 | Cu   | 10.163 | 4.475  | 1.926 |
| O    | 8.489  | 1.860 | 8.956  | Cu   | 1.456  | 3.521  | 4.874 | Cu   | 6.484  | 6.973  | 1.948 |
| S    | -0.227 | 0.277 | 9.607  | Cu   | 5.169  | 1.067  | 5.001 | Cu   | 4.645  | 2.921  | 1.926 |
|      |        |       |        | Cu   | 7.003  | 5.124  | 4.901 | Cu   | 10.063 | 6.976  | 1.397 |
|      |        |       |        | Cu   | 12.426 | 9.195  | 4.413 | Cu   | 8.221  | 2.915  | 1.392 |
| Pt   | 7.363  | 5.723 | 7.342  | Cu   | 10.573 | 5.100  | 4.348 | Cu   | 4.528  | 5.422  | 1.403 |
| Pt   | 1.855  | 4.093 | 7.268  | Cu   | 6.895  | 7.623  | 4.365 | Cu   | 2.688  | 1.349  | 1.394 |
| Cu   | 5.601  | 1.711 | 7.340  | Cu   | 5.049  | 3.561  | 4.353 | Cu   | 6.287  | 1.342  | 0.922 |
| Cu   | 0.106  | 0.177 | 7.346  | Cu   | 10.476 | 7.616  | 3.782 | Cu   | 8.112  | 5.400  | 0.887 |
| Cu   | 12.813 | 9.777 | 6.837  | Cu   | 8.639  | 3.552  | 3.773 | Cu   | 0.731  | -0.220 | 0.928 |
| Cu   | 10.962 | 5.738 | 6.698  | Cu   | 4.938  | 6.066  | 3.781 | Cu   | 2.588  | 3.851  | 0.924 |

**Table S53:** Coordinates for the most stable D- $\mu_3$ -cysteine adsorbed on Pt-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.418  | 4.297  | 9.949  | Cu   | 7.257  | 8.245  | 6.829 | Cu   | 3.046  | 1.996  | 3.859 |
| C    | 9.854  | 4.416  | 9.366  | Cu   | 5.349  | 4.202  | 6.737 | Cu   | 8.498  | 6.062  | 3.252 |
| C    | 7.803  | 3.022  | 9.358  | Cu   | 10.808 | 8.259  | 6.290 | Cu   | 6.624  | 2.015  | 3.269 |
| H    | 5.633  | 3.932  | 8.954  | Cu   | 9.028  | 4.163  | 6.216 | Cu   | 2.924  | 4.500  | 3.253 |
| H    | 8.301  | 2.136  | 9.772  | Cu   | 5.314  | 6.690  | 6.163 | Cu   | 1.105  | 0.457  | 3.277 |
| H    | 7.971  | 3.032  | 8.263  | Cu   | 3.472  | 2.594  | 6.271 | Cu   | 2.806  | 6.959  | 2.597 |
| H    | 8.467  | 4.230  | 11.051 | Cu   | 8.930  | 6.704  | 5.653 | Cu   | 0.946  | 2.908  | 2.614 |
| H    | 6.823  | 5.633  | 10.094 | Cu   | 7.067  | 2.645  | 5.660 | Cu   | 8.353  | 8.542  | 2.638 |
| H    | 8.299  | 6.325  | 9.723  | Cu   | 3.391  | 5.162  | 5.594 | Cu   | 6.510  | 4.461  | 2.564 |
| N    | 7.681  | 5.522  | 9.545  | Cu   | 1.507  | 1.083  | 5.708 | Cu   | 11.956 | 8.535  | 2.005 |
| O    | 10.236 | 5.564  | 8.995  | Cu   | -0.423 | -0.488 | 5.012 | Cu   | 10.130 | 4.479  | 2.029 |
| O    | -0.592 | 0.194  | 9.228  | Cu   | 1.375  | 3.528  | 5.000 | Cu   | 6.455  | 6.968  | 1.991 |
| S    | 6.008  | 2.752  | 9.565  | Cu   | 5.112  | 1.078  | 5.088 | Cu   | 4.576  | 2.930  | 1.991 |
|      |        |        |        | Cu   | 6.949  | 5.111  | 4.945 | Cu   | 10.005 | 6.981  | 1.466 |
|      |        |        |        | Cu   | 12.360 | 9.181  | 4.403 | Cu   | 8.175  | 2.918  | 1.453 |
| Pt   | 7.302  | 5.712  | 7.376  | Cu   | 10.546 | 5.133  | 4.489 | Cu   | 4.476  | 5.413  | 1.436 |
| Pt   | 1.862  | 4.222  | 7.363  | Cu   | 6.856  | 7.628  | 4.418 | Cu   | 2.639  | 1.357  | 1.477 |
| Cu   | 5.525  | 1.733  | 7.444  | Cu   | 4.992  | 3.551  | 4.399 | Cu   | 6.212  | 1.358  | 0.984 |
| Cu   | 0.053  | -0.048 | 7.377  | Cu   | 10.418 | 7.630  | 3.853 | Cu   | 8.092  | 5.393  | 0.949 |
| Cu   | 12.799 | 9.797  | 6.749  | Cu   | 8.595  | 3.549  | 3.830 | Cu   | 0.700  | -0.208 | 0.990 |
| Cu   | 10.922 | 5.754  | 6.971  | Cu   | 4.896  | 6.052  | 3.789 | Cu   | 2.515  | 3.838  | 0.977 |

**Table S54:** Coordinates for the most stable L- $\mu_3$ -cysteine adsorbed on Pt-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.479  | 5.334  | 9.929  | Cu   | 7.474  | 7.981 | 6.714 | Cu   | 3.172  | 1.758 | 3.751 |
| C    | 4.163  | 5.606  | 9.156  | Cu   | 5.422  | 3.959 | 6.677 | Cu   | 8.621  | 5.843 | 3.180 |
| C    | 5.900  | 3.870  | 9.970  | Cu   | 10.943 | 7.986 | 6.173 | Cu   | 6.739  | 1.774 | 3.113 |
| H    | 5.007  | 3.251  | 10.127 | Cu   | 9.137  | 3.973 | 6.167 | Cu   | 3.047  | 4.255 | 3.135 |
| H    | 6.610  | 3.701  | 10.795 | Cu   | 5.437  | 6.473 | 6.089 | Cu   | 1.231  | 0.218 | 3.177 |
| H    | 5.264  | 5.644  | 10.971 | Cu   | 3.573  | 2.330 | 6.156 | Cu   | 2.940  | 6.718 | 2.488 |
| H    | 7.313  | 6.315  | 10.062 | Cu   | 9.045  | 6.434 | 5.602 | Cu   | 1.100  | 2.686 | 2.522 |
| H    | 6.139  | 7.141  | 9.219  | Cu   | 7.221  | 2.393 | 5.431 | Cu   | 8.472  | 8.299 | 2.505 |
| N    | 6.552  | 6.214  | 9.384  | Cu   | 3.514  | 4.939 | 5.479 | Cu   | 6.637  | 4.234 | 2.508 |
| O    | 3.955  | 6.835  | 8.884  | Cu   | 1.655  | 0.816 | 5.601 | Cu   | 12.088 | 8.303 | 1.879 |
| O    | 3.408  | 4.613  | 8.943  | Cu   | 3.370  | 7.403 | 4.908 | Cu   | 10.269 | 4.252 | 1.908 |
| S    | 6.750  | 3.284  | 8.442  | Cu   | 1.530  | 3.321 | 4.920 | Cu   | 6.563  | 6.742 | 1.914 |
|      |        |        |        | Cu   | 8.942  | 8.947 | 4.936 | Cu   | 4.698  | 2.689 | 1.881 |
|      |        |        |        | Cu   | 7.091  | 4.870 | 4.919 | Cu   | 10.154 | 6.746 | 1.367 |
|      |        |        |        | Cu   | 12.496 | 8.939 | 4.282 | Cu   | 8.305  | 2.687 | 1.343 |
| Pt   | 7.416  | 5.494  | 7.419  | Cu   | 10.674 | 4.892 | 4.342 | Cu   | 4.611  | 5.174 | 1.353 |
| Pt   | 1.992  | 4.013  | 7.309  | Cu   | 6.985  | 7.391 | 4.327 | Cu   | 2.757  | 1.135 | 1.362 |
| Cu   | 5.730  | 1.546  | 7.246  | Cu   | 5.109  | 3.326 | 4.308 | Cu   | 10.032 | 9.230 | 0.846 |
| Cu   | 0.050  | -0.177 | 7.265  | Cu   | 10.544 | 7.386 | 3.749 | Cu   | 8.208  | 5.176 | 0.889 |
| Cu   | 12.860 | 9.588  | 6.644  | Cu   | 8.735  | 3.333 | 3.708 | Cu   | 4.515  | 7.667 | 0.885 |
| Cu   | 11.132 | 5.491  | 6.741  | Cu   | 5.029  | 5.822 | 3.726 | Cu   | 2.648  | 3.615 | 0.840 |

**Table S55:** Coordinates for the most stable D- $\mu_4$ -cysteine adsorbed on Pt-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.318  | 4.350  | 9.875  | Cu   | 7.275  | 8.280  | 6.793 | Cu   | 3.079  | 1.972  | 3.884 |
| C    | 9.765  | 4.421  | 9.326  | Cu   | 5.421  | 4.185  | 7.018 | Cu   | 8.515  | 6.035  | 3.259 |
| C    | 7.627  | 3.104  | 9.266  | Cu   | 10.849 | 8.243  | 6.268 | Cu   | 6.653  | 2.001  | 3.283 |
| H    | 7.896  | 2.225  | 9.865  | Cu   | 9.049  | 4.156  | 6.215 | Cu   | 2.956  | 4.476  | 3.299 |
| H    | 8.035  | 2.951  | 8.249  | Cu   | 5.343  | 6.666  | 6.193 | Cu   | 1.126  | 0.430  | 3.293 |
| H    | 8.349  | 4.252  | 10.976 | Cu   | 3.489  | 2.604  | 6.269 | Cu   | 2.839  | 6.940  | 2.625 |
| H    | 6.702  | 5.647  | 9.949  | Cu   | 8.979  | 6.711  | 5.615 | Cu   | 0.989  | 2.885  | 2.633 |
| H    | 8.195  | 6.407  | 9.827  | Cu   | 7.098  | 2.629  | 5.666 | Cu   | 8.377  | 8.501  | 2.624 |
| N    | 7.628  | 5.612  | 9.509  | Cu   | 3.463  | 5.135  | 5.667 | Cu   | 6.529  | 4.433  | 2.594 |
| O    | 10.194 | 5.552  | 8.940  | Cu   | 1.517  | 1.067  | 5.728 | Cu   | 12.002 | 8.515  | 2.019 |
| O    | 10.377 | 3.305  | 9.215  | Cu   | -0.392 | -0.508 | 5.045 | Cu   | 10.157 | 4.460  | 2.043 |
| S    | 5.798  | 3.138  | 9.068  | Cu   | 1.397  | 3.510  | 5.026 | Cu   | 6.464  | 6.941  | 2.006 |
|      |        |        |        | Cu   | 5.142  | 1.057  | 5.051 | Cu   | 4.605  | 2.899  | 2.051 |
|      |        |        |        | Cu   | 6.967  | 5.085  | 4.983 | Cu   | 10.040 | 6.956  | 1.474 |
|      |        |        |        | Cu   | 12.405 | 9.164  | 4.425 | Cu   | 8.209  | 2.898  | 1.471 |
| Pt   | 7.413  | 5.822  | 7.354  | Cu   | 10.575 | 5.114  | 4.490 | Cu   | 4.498  | 5.385  | 1.470 |
| Pt   | 1.876  | 4.206  | 7.389  | Cu   | 6.873  | 7.599  | 4.415 | Cu   | 2.660  | 1.333  | 1.499 |
| Cu   | 5.535  | 1.652  | 7.404  | Cu   | 5.040  | 3.560  | 4.499 | Cu   | 6.252  | 1.341  | 1.000 |
| Cu   | 0.079  | -0.067 | 7.420  | Cu   | 10.465 | 7.611  | 3.836 | Cu   | 8.103  | 5.367  | 0.968 |
| Cu   | 12.825 | 9.785  | 6.777  | Cu   | 8.623  | 3.528  | 3.847 | Cu   | 0.714  | -0.234 | 1.000 |
| Cu   | 10.938 | 5.733  | 6.987  | Cu   | 4.920  | 6.027  | 3.823 | Cu   | 2.563  | 3.810  | 1.006 |

**Table S56:** Coordinates for the most stable L- $\mu_4$ -cysteine adsorbed on Pt-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.423  | 5.150  | 9.978  | Cu   | 7.419  | 8.091 | 6.639 | Cu   | 3.197  | 1.823 | 3.723 |
| C    | 4.195  | 5.568  | 9.133  | Cu   | 5.523  | 3.956 | 6.607 | Cu   | 8.661  | 5.912 | 3.156 |
| C    | 5.746  | 3.666  | 9.948  | Cu   | 11.051 | 8.025 | 6.177 | Cu   | 6.802  | 1.849 | 3.129 |
| H    | 4.866  | 3.076  | 10.231 | Cu   | 9.223  | 4.005 | 6.148 | Cu   | 3.085  | 4.329 | 3.128 |
| H    | 6.580  | 3.434  | 10.630 | Cu   | 5.473  | 6.503 | 6.032 | Cu   | 1.249  | 0.283 | 3.143 |
| H    | 6.055  | 3.364  | 8.927  | Cu   | 3.607  | 2.424 | 6.119 | Cu   | 2.967  | 6.792 | 2.478 |
| H    | 5.159  | 5.436  | 11.017 | Cu   | 9.109  | 6.521 | 5.581 | Cu   | 1.130  | 2.762 | 2.533 |
| H    | 7.354  | 5.865  | 10.238 | Cu   | 7.240  | 2.466 | 5.515 | Cu   | 8.502  | 8.360 | 2.446 |
| H    | 6.322  | 6.935  | 9.486  | Cu   | 3.553  | 4.983 | 5.471 | Cu   | 6.669  | 4.304 | 2.472 |
| N    | 6.601  | 5.948  | 9.549  | Cu   | 1.669  | 0.881 | 5.564 | Cu   | 12.131 | 8.385 | 1.882 |
| O    | 4.131  | 6.817  | 8.874  | Cu   | 3.417  | 7.449 | 4.886 | Cu   | 10.306 | 4.325 | 1.895 |
| O    | 3.355  | 4.668  | 8.837  | Cu   | 1.599  | 3.397 | 4.980 | Cu   | 6.594  | 6.805 | 1.862 |
|      |        |        |        | Cu   | 8.971  | 8.968 | 4.847 | Cu   | 4.730  | 2.751 | 1.870 |
|      |        |        |        | Cu   | 7.142  | 4.934 | 4.888 | Cu   | 10.201 | 6.824 | 1.355 |
|      |        |        |        | Cu   | 12.534 | 9.004 | 4.293 | Cu   | 8.350  | 2.767 | 1.334 |
| Au   | 7.508  | 5.521  | 7.409  | Cu   | 10.707 | 4.960 | 4.325 | Cu   | 4.629  | 5.236 | 1.325 |
| Cu   | 5.682  | 1.481  | 7.126  | Cu   | 7.007  | 7.449 | 4.272 | Cu   | 2.763  | 1.200 | 1.350 |
| Cu   | 2.147  | 4.139  | 7.306  | Cu   | 5.150  | 3.379 | 4.270 | Cu   | 10.094 | 9.325 | 0.850 |
| Cu   | 0.125  | -0.189 | 7.264  | Cu   | 10.607 | 7.444 | 3.742 | Cu   | 8.259  | 5.258 | 0.867 |
| Cu   | 12.910 | 9.647  | 6.628  | Cu   | 8.763  | 3.395 | 3.711 | Cu   | 4.532  | 7.723 | 0.859 |
| Cu   | 11.178 | 5.542  | 6.720  | Cu   | 5.066  | 5.878 | 3.679 | Cu   | 2.667  | 3.684 | 0.846 |

**Table S57:** Coordinates for the most stable D-alanine adsorbed on Au-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.020  | 4.034 | 10.128 | Cu   | 7.127  | 8.207  | 6.675 | Cu   | 2.930  | 1.919  | 3.717 |
| C    | 8.902  | 3.175 | 9.203  | Cu   | 5.239  | 4.089  | 6.682 | Cu   | 8.355  | 5.999  | 3.143 |
| C    | 6.578  | 3.566 | 10.204 | Cu   | 10.715 | 8.159  | 6.126 | Cu   | 6.523  | 1.939  | 3.151 |
| H    | 5.978  | 4.250 | 10.825 | Cu   | 8.927  | 4.100  | 6.048 | Cu   | 2.831  | 4.444  | 3.159 |
| H    | 6.526  | 2.556 | 10.631 | Cu   | 5.164  | 6.628  | 6.154 | Cu   | 0.962  | 0.371  | 3.149 |
| H    | 6.141  | 3.534 | 9.189  | Cu   | 3.336  | 2.542  | 6.128 | Cu   | 2.687  | 6.899  | 2.500 |
| H    | 8.482  | 4.018 | 11.133 | Cu   | 8.804  | 6.647  | 5.517 | Cu   | 0.839  | 2.825  | 2.466 |
| H    | 7.597  | 6.072 | 10.203 | Cu   | 6.967  | 2.579  | 5.528 | Cu   | 8.230  | 8.449  | 2.475 |
| H    | 9.065  | 5.707 | 9.503  | Cu   | 3.247  | 5.078  | 5.566 | Cu   | 6.382  | 4.401  | 2.508 |
| N    | 8.082  | 5.419 | 9.580  | Cu   | 1.397  | 1.001  | 5.551 | Cu   | 11.867 | 8.472  | 1.924 |
| O    | 10.090 | 3.617 | 9.021  | Cu   | -0.548 | -0.585 | 4.951 | Cu   | 10.000 | 4.404  | 1.866 |
| O    | 8.384  | 2.160 | 8.652  | Cu   | 1.299  | 3.464  | 4.855 | Cu   | 6.306  | 6.904  | 1.892 |
|      |        |       |        | Cu   | 4.985  | 0.973  | 4.872 | Cu   | 4.477  | 2.844  | 1.889 |
|      |        |       |        | Cu   | 6.825  | 5.056  | 4.914 | Cu   | 9.901  | 6.904  | 1.348 |
|      |        |       |        | Cu   | 12.282 | 9.128  | 4.373 | Cu   | 8.050  | 2.849  | 1.341 |
| Au   | 7.257  | 5.636 | 7.396  | Cu   | 10.415 | 5.043  | 4.275 | Cu   | 4.360  | 5.345  | 1.361 |
| Cu   | 5.399  | 1.627 | 7.159  | Cu   | 6.710  | 7.554  | 4.301 | Cu   | 2.512  | 1.280  | 1.352 |
| Cu   | 1.679  | 4.053 | 7.156  | Cu   | 4.871  | 3.490  | 4.311 | Cu   | 6.132  | 1.274  | 0.867 |
| Cu   | -0.089 | 0.106 | 7.289  | Cu   | 10.328 | 7.547  | 3.714 | Cu   | 7.944  | 5.335  | 0.861 |
| Cu   | 12.651 | 9.691 | 6.794  | Cu   | 8.474  | 3.482  | 3.705 | Cu   | 0.561  | -0.289 | 0.861 |
| Cu   | 10.825 | 5.692 | 6.626  | Cu   | 4.772  | 5.988  | 3.737 | Cu   | 2.422  | 3.784  | 0.874 |

**Table S58:** Coordinates for the most stable L-alanine adsorbed on Au-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.171  | 3.774 | 9.992  | Cu   | 7.270  | 8.316  | 6.737 | Cu   | 3.075  | 2.068  | 3.756 |
| C    | 7.685  | 2.551 | 9.187  | Cu   | 5.370  | 4.221  | 6.689 | Cu   | 8.494  | 6.157  | 3.200 |
| C    | 9.612  | 4.255 | 9.690  | Cu   | 10.866 | 8.264  | 6.151 | Cu   | 6.653  | 2.081  | 3.184 |
| H    | 10.010 | 4.792 | 10.568 | Cu   | 9.067  | 4.198  | 6.152 | Cu   | 2.972  | 4.592  | 3.189 |
| H    | 9.947  | 2.383 | 9.237  | Cu   | 5.318  | 6.746  | 6.173 | Cu   | 1.106  | 0.534  | 3.202 |
| H    | 9.558  | 4.961 | 8.840  | Cu   | 3.501  | 2.647  | 6.171 | Cu   | 2.828  | 7.051  | 2.540 |
| H    | 8.124  | 3.445 | 11.050 | Cu   | 8.928  | 6.759  | 5.606 | Cu   | 0.973  | 2.984  | 2.500 |
| H    | 7.388  | 5.655 | 10.430 | Cu   | 7.097  | 2.701  | 5.561 | Cu   | 8.378  | 8.623  | 2.540 |
| H    | 6.286  | 4.567 | 9.816  | Cu   | 3.394  | 5.199  | 5.589 | Cu   | 6.524  | 4.555  | 2.548 |
| N    | 7.252  | 4.904 | 9.748  | Cu   | 1.549  | 1.137  | 5.600 | Cu   | 11.989 | 8.627  | 1.956 |
| O    | 6.445  | 2.478 | 8.950  | Cu   | -0.408 | -0.450 | 4.985 | Cu   | 10.135 | 4.562  | 1.922 |
| O    | 12.259 | 9.789 | 8.868  | Cu   | 1.436  | 3.595  | 4.891 | Cu   | 6.458  | 7.076  | 1.937 |
| O    | -0.539 | 0.080 | 9.354  | Cu   | 5.137  | 1.121  | 4.975 | Cu   | 4.617  | 3.012  | 1.921 |
|      |        |       |        | Cu   | 6.981  | 5.179  | 4.951 | Cu   | 10.026 | 7.070  | 1.389 |
|      |        |       |        | Cu   | 12.409 | 9.255  | 4.379 | Cu   | 8.186  | 3.002  | 1.387 |
| Au   | 7.380  | 5.746 | 7.470  | Cu   | 10.542 | 5.184  | 4.332 | Cu   | 4.514  | 5.515  | 1.394 |
| Cu   | 5.577  | 1.713 | 7.297  | Cu   | 6.858  | 7.701  | 4.350 | Cu   | 2.661  | 1.452  | 1.390 |
| Cu   | 1.839  | 4.154 | 7.183  | Cu   | 5.015  | 3.625  | 4.343 | Cu   | 6.255  | 1.437  | 0.894 |
| Cu   | 0.074  | 0.196 | 7.317  | Cu   | 10.447 | 7.683  | 3.765 | Cu   | 8.082  | 5.494  | 0.917 |
| Cu   | 12.797 | 9.804 | 6.764  | Cu   | 8.611  | 3.628  | 3.759 | Cu   | 0.708  | -0.117 | 0.919 |
| Cu   | 10.966 | 5.794 | 6.685  | Cu   | 4.921  | 6.135  | 3.771 | Cu   | 2.564  | 3.963  | 0.909 |

**Table S59:** Coordinates for the most stable D- $\mu_3$ -serine adsorbed on Au-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 9.382  | 5.981  | 9.914  | Cu   | 7.068  | 8.050 | 6.689 | Cu   | 2.941  | 1.770 | 3.757 |
| C    | 10.236 | 7.035  | 9.167  | Cu   | 5.267  | 3.859 | 6.773 | Cu   | 8.335  | 5.827 | 3.182 |
| C    | 9.642  | 4.482  | 9.610  | Cu   | 10.781 | 8.031 | 6.027 | Cu   | 6.511  | 1.781 | 3.214 |
| H    | 0.389  | 1.881  | 9.102  | Cu   | 8.906  | 3.941 | 6.134 | Cu   | 2.845  | 4.289 | 3.181 |
| H    | 9.373  | 3.881  | 10.494 | Cu   | 5.117  | 6.438 | 6.200 | Cu   | 0.977  | 0.220 | 3.169 |
| H    | 8.968  | 4.195  | 8.779  | Cu   | 3.346  | 2.380 | 6.245 | Cu   | 2.701  | 6.752 | 2.521 |
| H    | 9.618  | 6.164  | 10.981 | Cu   | 8.800  | 6.514 | 5.535 | Cu   | 0.850  | 2.670 | 2.488 |
| H    | 7.351  | 5.832  | 10.359 | Cu   | 6.943  | 2.400 | 5.615 | Cu   | 8.226  | 8.288 | 2.550 |
| H    | 7.806  | 7.263  | 9.634  | Cu   | 3.232  | 4.865 | 5.645 | Cu   | 6.378  | 4.248 | 2.575 |
| N    | 7.953  | 6.246  | 9.644  | Cu   | 1.413  | 0.863 | 5.547 | Cu   | 11.872 | 8.296 | 1.914 |
| O    | 9.701  | 8.148  | 8.921  | Cu   | 3.165  | 7.398 | 4.970 | Cu   | 9.990  | 4.246 | 1.893 |
| O    | 11.464 | 6.699  | 8.944  | Cu   | 1.343  | 3.321 | 4.906 | Cu   | 6.305  | 6.751 | 1.935 |
| O    | -0.089 | 1.009  | 9.237  | Cu   | 4.973  | 0.844 | 4.961 | Cu   | 4.489  | 2.690 | 1.942 |
|      |        |        |        | Cu   | 6.814  | 4.883 | 4.985 | Cu   | 9.880  | 6.728 | 1.370 |
|      |        |        |        | Cu   | 12.300 | 8.964 | 4.318 | Cu   | 8.029  | 2.686 | 1.401 |
| Au   | 7.238  | 5.529  | 7.437  | Cu   | 10.403 | 4.884 | 4.273 | Cu   | 4.380  | 5.196 | 1.391 |
| Cu   | 5.463  | 1.257  | 7.328  | Cu   | 6.696  | 7.380 | 4.342 | Cu   | 2.537  | 1.126 | 1.381 |
| Cu   | 1.607  | 3.968  | 7.296  | Cu   | 4.861  | 3.333 | 4.379 | Cu   | 9.804  | 9.210 | 0.933 |
| Cu   | -0.084 | -0.022 | 7.303  | Cu   | 10.325 | 7.374 | 3.714 | Cu   | 7.920  | 5.172 | 0.898 |
| Cu   | 12.708 | 9.597  | 6.697  | Cu   | 8.462  | 3.325 | 3.763 | Cu   | 4.272  | 7.691 | 0.887 |
| Cu   | 10.812 | 5.526  | 6.547  | Cu   | 4.757  | 5.824 | 3.790 | Cu   | 2.448  | 3.615 | 0.901 |

**Table S60:** Coordinates for the most stable L- $\mu_3$ -serine adsorbed on Au-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.312  | 4.953  | 9.890  | Cu   | 7.452  | 8.121 | 6.673 | Cu   | 3.223  | 1.854 | 3.755 |
| C    | 4.105  | 5.516  | 9.104  | Cu   | 5.521  | 4.028 | 6.712 | Cu   | 8.663  | 5.929 | 3.183 |
| C    | 5.541  | 3.446  | 9.710  | Cu   | 11.020 | 8.060 | 6.186 | Cu   | 6.801  | 1.864 | 3.148 |
| H    | 4.599  | 2.946  | 9.997  | Cu   | 9.236  | 4.019 | 6.160 | Cu   | 3.106  | 4.350 | 3.146 |
| H    | 6.326  | 3.139  | 10.433 | Cu   | 5.505  | 6.523 | 6.068 | Cu   | 1.278  | 0.313 | 3.168 |
| H    | 5.039  | 5.091  | 10.957 | Cu   | 3.613  | 2.446 | 6.129 | Cu   | 2.988  | 6.813 | 2.493 |
| H    | 7.235  | 5.598  | 10.308 | Cu   | 9.106  | 6.528 | 5.593 | Cu   | 1.152  | 2.780 | 2.539 |
| H    | 6.258  | 6.744  | 9.596  | Cu   | 7.253  | 2.480 | 5.505 | Cu   | 8.531  | 8.394 | 2.514 |
| N    | 6.525  | 5.752  | 9.587  | Cu   | 3.571  | 5.001 | 5.497 | Cu   | 6.677  | 4.322 | 2.502 |
| O    | 4.145  | 6.768  | 8.863  | Cu   | 1.685  | 0.901 | 5.597 | Cu   | 12.138 | 8.400 | 1.900 |
| O    | 3.159  | 4.712  | 8.845  | Cu   | 3.440  | 7.469 | 4.904 | Cu   | 10.324 | 4.338 | 1.911 |
| O    | 5.952  | 3.091  | 8.415  | Cu   | 1.596  | 3.416 | 4.981 | Cu   | 6.620  | 6.834 | 1.893 |
|      |        |        |        | Cu   | 9.001  | 9.018 | 4.941 | Cu   | 4.750  | 2.787 | 1.914 |
|      |        |        |        | Cu   | 7.142  | 4.946 | 4.929 | Cu   | 10.201 | 6.846 | 1.383 |
|      |        |        |        | Cu   | 12.553 | 9.017 | 4.307 | Cu   | 8.355  | 2.776 | 1.360 |
| Au   | 7.580  | 5.595  | 7.458  | Cu   | 10.725 | 4.979 | 4.334 | Cu   | 4.650  | 5.266 | 1.346 |
| Cu   | 5.712  | 1.519  | 7.268  | Cu   | 7.027  | 7.477 | 4.306 | Cu   | 2.807  | 1.226 | 1.376 |
| Cu   | 2.081  | 4.125  | 7.285  | Cu   | 5.178  | 3.423 | 4.340 | Cu   | 10.085 | 9.345 | 0.867 |
| Cu   | 0.134  | -0.180 | 7.288  | Cu   | 10.610 | 7.467 | 3.762 | Cu   | 8.265  | 5.261 | 0.899 |
| Cu   | 12.920 | 9.659  | 6.633  | Cu   | 8.776  | 3.417 | 3.728 | Cu   | 4.569  | 7.750 | 0.880 |
| Cu   | 11.176 | 5.559  | 6.733  | Cu   | 5.084  | 5.907 | 3.707 | Cu   | 2.698  | 3.709 | 0.859 |

**Table S61:** Coordinates for the most stable D- $\mu_4$ -serine adsorbed on Au-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 9.514  | 6.120  | 9.890  | Cu   | 7.057  | 8.002 | 6.658 | Cu   | 2.877  | 1.739 | 3.769 |
| C    | 10.229 | 7.296  | 9.183  | Cu   | 5.249  | 3.843 | 6.745 | Cu   | 8.304  | 5.795 | 3.165 |
| C    | 10.163 | 4.753  | 9.648  | Cu   | 10.708 | 7.971 | 6.027 | Cu   | 6.459  | 1.751 | 3.170 |
| H    | 0.089  | 1.669  | 10.109 | Cu   | 8.826  | 3.864 | 6.089 | Cu   | 2.772  | 4.249 | 3.196 |
| H    | 9.562  | 3.995  | 10.193 | Cu   | 5.111  | 6.380 | 6.176 | Cu   | 0.923  | 0.188 | 3.164 |
| H    | 9.638  | 6.323  | 10.975 | Cu   | 3.290  | 2.364 | 6.243 | Cu   | 2.650  | 6.704 | 2.484 |
| H    | 7.548  | 5.592  | 10.260 | Cu   | 8.778  | 6.460 | 5.517 | Cu   | 0.795  | 2.649 | 2.511 |
| H    | 7.745  | 7.107  | 9.599  | Cu   | 6.883  | 2.359 | 5.556 | Cu   | 8.180  | 8.265 | 2.527 |
| N    | 8.065  | 6.131  | 9.560  | Cu   | 3.182  | 4.836 | 5.645 | Cu   | 6.348  | 4.214 | 2.559 |
| O    | 9.496  | 8.304  | 8.913  | Cu   | 1.350  | 0.798 | 5.564 | Cu   | 11.801 | 8.273 | 1.890 |
| O    | 11.481 | 7.181  | 8.995  | Cu   | 3.115  | 7.320 | 4.921 | Cu   | 9.955  | 4.225 | 1.906 |
| O    | 10.239 | 4.402  | 8.290  | Cu   | 1.261  | 3.266 | 4.967 | Cu   | 6.267  | 6.719 | 1.913 |
|      |        |        |        | Cu   | 8.619  | 8.931 | 4.936 | Cu   | 4.430  | 2.663 | 1.937 |
|      |        |        |        | Cu   | 6.785  | 4.856 | 4.970 | Cu   | 9.832  | 6.708 | 1.355 |
|      |        |        |        | Cu   | 12.227 | 8.916 | 4.287 | Cu   | 7.989  | 2.661 | 1.375 |
| Au   | 7.248  | 5.473  | 7.445  | Cu   | 10.378 | 4.860 | 4.340 | Cu   | 4.334  | 5.158 | 1.387 |
| Cu   | 5.428  | 1.298  | 7.298  | Cu   | 6.661  | 7.345 | 4.322 | Cu   | 2.482  | 1.106 | 1.386 |
| Cu   | 1.571  | 3.992  | 7.349  | Cu   | 4.813  | 3.303 | 4.361 | Cu   | 9.741  | 9.190 | 0.886 |
| Cu   | -0.180 | -0.259 | 7.271  | Cu   | 10.274 | 7.343 | 3.704 | Cu   | 7.892  | 5.141 | 0.877 |
| Cu   | 12.605 | 9.532  | 6.646  | Cu   | 8.434  | 3.292 | 3.738 | Cu   | 4.228  | 7.667 | 0.878 |
| Cu   | 10.793 | 5.487  | 6.710  | Cu   | 4.724  | 5.779 | 3.763 | Cu   | 2.383  | 3.593 | 0.909 |

**Table S62:** Coordinates for the most stable L- $\mu_4$ -serine adsorbed on Au-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.103  | 3.914  | 9.994  | Cu   | 7.278  | 8.323  | 6.719 | Cu   | 3.096  | 2.029  | 3.741 |
| C    | 7.646  | 2.679  | 9.176  | Cu   | 5.374  | 4.218  | 6.669 | Cu   | 8.511  | 6.104  | 3.194 |
| C    | 9.507  | 4.497  | 9.743  | Cu   | 10.874 | 8.260  | 6.159 | Cu   | 6.669  | 2.032  | 3.184 |
| H    | 9.752  | 5.186  | 10.566 | Cu   | 9.072  | 4.195  | 6.153 | Cu   | 2.986  | 4.545  | 3.189 |
| H    | -1.067 | -0.865 | 9.393  | Cu   | 5.314  | 6.741  | 6.145 | Cu   | 1.120  | 0.475  | 3.189 |
| H    | 9.481  | 5.078  | 8.804  | Cu   | 3.506  | 2.641  | 6.154 | Cu   | 2.838  | 6.996  | 2.540 |
| H    | 8.047  | 3.583  | 11.051 | Cu   | 8.941  | 6.741  | 5.595 | Cu   | 0.990  | 2.920  | 2.507 |
| H    | 7.266  | 5.783  | 10.396 | Cu   | 7.110  | 2.683  | 5.555 | Cu   | 8.394  | 8.559  | 2.538 |
| H    | 6.191  | 4.658  | 9.779  | Cu   | 3.396  | 5.188  | 5.583 | Cu   | 6.537  | 4.499  | 2.539 |
| N    | 7.151  | 5.015  | 9.728  | Cu   | 1.565  | 1.124  | 5.562 | Cu   | 12.008 | 8.562  | 1.967 |
| O    | 6.404  | 2.603  | 8.929  | Cu   | -0.407 | -0.467 | 4.986 | Cu   | 10.155 | 4.494  | 1.917 |
| O    | 12.206 | 9.908  | 8.861  | Cu   | 1.449  | 3.573  | 4.884 | Cu   | 6.473  | 7.006  | 1.929 |
| S    | -0.172 | 0.191  | 9.594  | Cu   | 5.153  | 1.097  | 4.971 | Cu   | 4.640  | 2.946  | 1.912 |
|      |        |        |        | Cu   | 6.991  | 5.148  | 4.934 | Cu   | 10.051 | 6.999  | 1.393 |
|      |        |        |        | Cu   | 12.421 | 9.227  | 4.389 | Cu   | 8.197  | 2.936  | 1.385 |
| Au   | 7.365  | 5.770  | 7.436  | Cu   | 10.557 | 5.144  | 4.326 | Cu   | 4.519  | 5.448  | 1.391 |
| Cu   | 5.581  | 1.724  | 7.296  | Cu   | 6.874  | 7.663  | 4.337 | Cu   | 2.678  | 1.378  | 1.385 |
| Cu   | 1.849  | 4.149  | 7.177  | Cu   | 5.029  | 3.590  | 4.333 | Cu   | 6.274  | 1.360  | 0.899 |
| Cu   | 0.109  | 0.212  | 7.314  | Cu   | 10.461 | 7.643  | 3.769 | Cu   | 8.107  | 5.425  | 0.913 |
| Cu   | 12.804 | 9.806  | 6.789  | Cu   | 8.625  | 3.589  | 3.754 | Cu   | 0.722  | -0.191 | 0.910 |
| Cu   | 10.982 | 5.789  | 6.667  | Cu   | 4.929  | 6.093  | 3.761 | Cu   | 2.576  | 3.887  | 0.916 |

**Table S63:** Coordinates for the most stable D- $\mu_3$ -cysteine adsorbed on Au-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 5.046  | 4.927 | 9.871  | Cu   | 7.453  | 8.325  | 6.708 | Cu   | 3.265  | 2.052  | 3.742 |
| C    | 4.490  | 3.590 | 9.289  | Cu   | 5.599  | 4.228  | 6.571 | Cu   | 8.707  | 6.154  | 3.219 |
| C    | 4.245  | 6.044 | 9.204  | Cu   | 11.093 | 8.291  | 6.280 | Cu   | 6.853  | 2.070  | 3.189 |
| H    | 3.208  | 6.025 | 9.564  | Cu   | 9.223  | 4.209  | 6.214 | Cu   | 3.133  | 4.562  | 3.194 |
| H    | 6.020  | 7.606 | 8.800  | Cu   | 5.500  | 6.785  | 6.089 | Cu   | 1.290  | 0.509  | 3.209 |
| H    | 4.211  | 5.850 | 8.117  | Cu   | 3.702  | 2.657  | 6.083 | Cu   | 3.012  | 7.029  | 2.568 |
| H    | 4.839  | 4.923 | 10.959 | Cu   | 9.112  | 6.757  | 5.663 | Cu   | 1.171  | 2.976  | 2.591 |
| H    | 6.954  | 5.589 | 10.354 | Cu   | 7.289  | 2.670  | 5.608 | Cu   | 8.572  | 8.606  | 2.536 |
| H    | 6.882  | 4.068 | 9.667  | Cu   | 3.574  | 5.200  | 5.569 | Cu   | 6.708  | 4.531  | 2.499 |
| N    | 6.502  | 5.022 | 9.633  | Cu   | 1.742  | 1.172  | 5.583 | Cu   | 12.175 | 8.607  | 1.963 |
| O    | 5.351  | 2.661 | 9.108  | Cu   | -0.233 | -0.428 | 4.984 | Cu   | 10.348 | 4.549  | 1.963 |
| O    | 3.252  | 3.534 | 9.025  | Cu   | 1.626  | 3.639  | 5.009 | Cu   | 6.641  | 7.038  | 1.935 |
| S    | 4.798  | 7.770 | 9.406  | Cu   | 5.368  | 1.108  | 4.991 | Cu   | 4.786  | 2.980  | 1.894 |
|      |        |       |        | Cu   | 7.187  | 5.171  | 4.909 | Cu   | 10.251 | 7.055  | 1.429 |
|      |        |       |        | Cu   | 12.581 | 9.237  | 4.370 | Cu   | 8.400  | 2.989  | 1.395 |
| Au   | 7.502  | 5.767 | 7.477  | Cu   | 10.729 | 5.185  | 4.391 | Cu   | 4.663  | 5.473  | 1.390 |
| Cu   | 5.692  | 1.752 | 7.340  | Cu   | 7.064  | 7.702  | 4.332 | Cu   | 2.817  | 1.414  | 1.394 |
| Cu   | 2.157  | 4.121 | 7.372  | Cu   | 5.211  | 3.604  | 4.284 | Cu   | 6.452  | 1.430  | 0.902 |
| Cu   | 0.208  | 0.270 | 7.320  | Cu   | 10.643 | 7.674  | 3.828 | Cu   | 8.315  | 5.492  | 0.935 |
| Cu   | 13.019 | 9.828 | 6.734  | Cu   | 8.795  | 3.622  | 3.778 | Cu   | 0.881  | -0.163 | 0.926 |
| Cu   | 11.157 | 5.828 | 6.743  | Cu   | 5.104  | 6.107  | 3.752 | Cu   | 2.707  | 3.903  | 0.918 |

**Table S64:** Coordinates for the most stable L- $\mu_3$ -cysteine adsorbed on Au-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.297  | 5.224  | 9.973  | Cu   | 7.442  | 8.053 | 6.659 | Cu   | 3.214  | 1.795 | 3.727 |
| C    | 4.059  | 5.555  | 9.104  | Cu   | 5.505  | 3.943 | 6.699 | Cu   | 8.656  | 5.876 | 3.175 |
| C    | 5.674  | 3.741  | 10.023 | Cu   | 11.033 | 8.007 | 6.164 | Cu   | 6.779  | 1.798 | 3.102 |
| H    | 4.755  | 3.158  | 10.162 | Cu   | 9.199  | 3.989 | 6.122 | Cu   | 3.094  | 4.288 | 3.117 |
| H    | 6.339  | 3.569  | 10.885 | Cu   | 5.475  | 6.478 | 6.041 | Cu   | 1.270  | 0.256 | 3.147 |
| H    | 4.970  | 5.490  | 11.000 | Cu   | 3.611  | 2.377 | 6.113 | Cu   | 2.970  | 6.747 | 2.462 |
| H    | 7.136  | 6.127  | 10.319 | Cu   | 9.096  | 6.487 | 5.596 | Cu   | 1.139  | 2.722 | 2.523 |
| H    | 6.070  | 7.041  | 9.421  | Cu   | 7.244  | 2.407 | 5.438 | Cu   | 8.512  | 8.331 | 2.482 |
| N    | 6.428  | 6.093  | 9.581  | Cu   | 3.568  | 4.938 | 5.470 | Cu   | 6.662  | 4.262 | 2.485 |
| O    | 3.912  | 6.793  | 8.839  | Cu   | 1.679  | 0.854 | 5.570 | Cu   | 12.119 | 8.335 | 1.877 |
| O    | 3.274  | 4.603  | 8.815  | Cu   | 3.418  | 7.418 | 4.869 | Cu   | 10.315 | 4.274 | 1.898 |
| S    | 6.588  | 3.112  | 8.563  | Cu   | 1.596  | 3.364 | 4.962 | Cu   | 6.609  | 6.775 | 1.874 |
|      |        |        |        | Cu   | 8.985  | 8.962 | 4.911 | Cu   | 4.738  | 2.723 | 1.871 |
|      |        |        |        | Cu   | 7.121  | 4.899 | 4.907 | Cu   | 10.188 | 6.778 | 1.368 |
|      |        |        |        | Cu   | 12.547 | 8.958 | 4.276 | Cu   | 8.335  | 2.710 | 1.333 |
| Au   | 7.528  | 5.553  | 7.462  | Cu   | 10.712 | 4.926 | 4.321 | Cu   | 4.641  | 5.203 | 1.322 |
| Cu   | 5.704  | 1.478  | 7.241  | Cu   | 7.016  | 7.419 | 4.286 | Cu   | 2.789  | 1.170 | 1.347 |
| Cu   | 2.105  | 4.078  | 7.275  | Cu   | 5.160  | 3.362 | 4.308 | Cu   | 10.066 | 9.263 | 0.826 |
| Cu   | 0.115  | -0.180 | 7.230  | Cu   | 10.596 | 7.412 | 3.748 | Cu   | 8.254  | 5.197 | 0.891 |
| Cu   | 12.910 | 9.614  | 6.603  | Cu   | 8.758  | 3.364 | 3.697 | Cu   | 4.555  | 7.689 | 0.862 |
| Cu   | 11.169 | 5.517  | 6.713  | Cu   | 5.066  | 5.853 | 3.681 | Cu   | 2.683  | 3.653 | 0.832 |

**Table S65:** Coordinates for the most stable D- $\mu_4$ -cysteine adsorbed on Au-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.374  | 4.269  | 9.938  | Cu   | 7.238  | 8.324  | 6.746 | Cu   | 3.064  | 2.002  | 3.868 |
| C    | 9.794  | 4.376  | 9.329  | Cu   | 5.374  | 4.144  | 7.017 | Cu   | 8.497  | 6.065  | 3.257 |
| C    | 7.660  | 3.064  | 9.258  | Cu   | 10.863 | 8.243  | 6.253 | Cu   | 6.647  | 2.022  | 3.271 |
| H    | 7.930  | 2.149  | 9.799  | Cu   | 9.063  | 4.148  | 6.186 | Cu   | 2.949  | 4.497  | 3.293 |
| H    | 8.055  | 2.967  | 8.227  | Cu   | 5.332  | 6.664  | 6.153 | Cu   | 1.114  | 0.458  | 3.275 |
| H    | 8.462  | 4.072  | 11.022 | Cu   | 3.455  | 2.632  | 6.251 | Cu   | 2.831  | 6.955  | 2.597 |
| H    | 6.743  | 5.530  | 10.149 | Cu   | 8.971  | 6.731  | 5.622 | Cu   | 0.975  | 2.906  | 2.611 |
| H    | 8.221  | 6.327  | 10.039 | Cu   | 7.092  | 2.635  | 5.651 | Cu   | 8.374  | 8.532  | 2.618 |
| N    | 7.663  | 5.539  | 9.697  | Cu   | 3.441  | 5.129  | 5.675 | Cu   | 6.527  | 4.465  | 2.611 |
| O    | 10.183 | 5.512  | 8.912  | Cu   | 1.485  | 1.087  | 5.704 | Cu   | 11.982 | 8.536  | 2.003 |
| O    | -0.655 | 0.150  | 9.203  | Cu   | -0.399 | -0.514 | 5.013 | Cu   | 10.148 | 4.481  | 2.028 |
| S    | 5.829  | 3.118  | 9.079  | Cu   | 1.387  | 3.522  | 5.039 | Cu   | 6.460  | 6.973  | 1.987 |
|      |        |        |        | Cu   | 5.138  | 1.074  | 5.039 | Cu   | 4.606  | 2.932  | 2.054 |
|      |        |        |        | Cu   | 6.975  | 5.097  | 5.016 | Cu   | 10.026 | 6.977  | 1.460 |
|      |        |        |        | Cu   | 12.399 | 9.167  | 4.410 | Cu   | 8.195  | 2.914  | 1.460 |
| Au   | 7.396  | 5.836  | 7.443  | Cu   | 10.558 | 5.139  | 4.474 | Cu   | 4.501  | 5.411  | 1.453 |
| Cu   | 5.527  | 1.642  | 7.392  | Cu   | 6.861  | 7.625  | 4.393 | Cu   | 2.662  | 1.365  | 1.488 |
| Cu   | 1.860  | 4.214  | 7.296  | Cu   | 5.034  | 3.585  | 4.507 | Cu   | 6.233  | 1.364  | 0.983 |
| Cu   | 0.071  | -0.083 | 7.387  | Cu   | 10.453 | 7.626  | 3.824 | Cu   | 8.098  | 5.387  | 0.972 |
| Cu   | 12.813 | 9.766  | 6.748  | Cu   | 8.617  | 3.548  | 3.827 | Cu   | 0.709  | -0.199 | 0.983 |
| Cu   | 10.956 | 5.754  | 6.977  | Cu   | 4.917  | 6.042  | 3.797 | Cu   | 2.567  | 3.848  | 1.004 |

**Table S66:** Coordinates for the most stable L- $\mu_4$ -cysteine adsorbed on Au-25%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 7.966  | 3.956 | 10.072 | Cu   | 7.320  | 8.275  | 6.688 | Cu   | 3.097  | 1.991  | 3.720 |
| C    | 7.717  | 2.756 | 9.135  | Cu   | 5.416  | 4.183  | 6.632 | Cu   | 8.515  | 6.060  | 3.137 |
| C    | 9.406  | 4.441 | 10.059 | Cu   | 10.859 | 8.201  | 6.119 | Cu   | 6.662  | 1.987  | 3.124 |
| H    | 9.528  | 5.323 | 10.708 | Cu   | 9.052  | 4.144  | 6.077 | Cu   | 2.976  | 4.501  | 3.150 |
| H    | 10.080 | 3.647 | 10.406 | Cu   | 5.334  | 6.704  | 6.123 | Cu   | 1.123  | 0.439  | 3.157 |
| H    | 9.699  | 4.720 | 9.031  | Cu   | 3.581  | 2.568  | 6.113 | Cu   | 2.830  | 6.941  | 2.464 |
| H    | 7.686  | 3.629 | 11.093 | Cu   | 8.942  | 6.688  | 5.532 | Cu   | 0.990  | 2.888  | 2.464 |
| H    | 7.127  | 5.850 | 10.267 | Cu   | 7.107  | 2.635  | 5.490 | Cu   | 8.397  | 8.526  | 2.501 |
| H    | 6.092  | 4.707 | 9.635  | Cu   | 3.420  | 5.154  | 5.537 | Cu   | 6.542  | 4.460  | 2.488 |
| N    | 7.059  | 5.049 | 9.633  | Cu   | 1.583  | 1.070  | 5.545 | Cu   | 11.993 | 8.522  | 1.910 |
| O    | 6.489  | 2.483 | 8.908  | Cu   | -0.426 | -0.543 | 4.884 | Cu   | 10.154 | 4.455  | 1.874 |
| O    | 8.734  | 2.162 | 8.672  | Cu   | 1.443  | 3.518  | 4.855 | Cu   | 6.482  | 6.971  | 1.888 |
|      |        |       |        | Cu   | 5.174  | 1.052  | 4.935 | Cu   | 4.630  | 2.913  | 1.872 |
|      |        |       |        | Cu   | 6.995  | 5.118  | 4.892 | Cu   | 10.044 | 6.966  | 1.346 |
|      |        |       |        | Cu   | 12.411 | 9.176  | 4.340 | Cu   | 8.190  | 2.897  | 1.324 |
| Au   | 7.431  | 5.729 | 7.411  | Cu   | 10.566 | 5.103  | 4.291 | Cu   | 4.526  | 5.408  | 1.350 |
| Au   | 1.884  | 4.053 | 7.354  | Cu   | 6.882  | 7.627  | 4.301 | Cu   | 2.680  | 1.351  | 1.358 |
| Cu   | 5.651  | 1.691 | 7.285  | Cu   | 5.033  | 3.557  | 4.288 | Cu   | 6.259  | 1.327  | 0.837 |
| Cu   | 0.027  | 0.145 | 7.164  | Cu   | 10.467 | 7.595  | 3.730 | Cu   | 8.104  | 5.383  | 0.853 |
| Cu   | 12.789 | 9.778 | 6.753  | Cu   | 8.620  | 3.542  | 3.692 | Cu   | 0.735  | -0.222 | 0.872 |
| Cu   | 10.926 | 5.702 | 6.677  | Cu   | 4.937  | 6.052  | 3.720 | Cu   | 2.573  | 3.864  | 0.862 |

**Table S67:** Coordinates for the most stable D-alanine adsorbed on Au-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.025  | 4.035 | 10.135 | Cu   | 7.128  | 8.200  | 6.678 | Cu   | 2.927  | 1.919  | 3.708 |
| C    | 8.903  | 3.183 | 9.203  | Cu   | 5.245  | 4.087  | 6.681 | Cu   | 8.352  | 5.998  | 3.135 |
| C    | 6.583  | 3.566 | 10.209 | Cu   | 10.696 | 8.164  | 6.118 | Cu   | 6.516  | 1.939  | 3.141 |
| H    | 5.981  | 4.246 | 10.832 | Cu   | 8.922  | 4.094  | 6.042 | Cu   | 2.827  | 4.446  | 3.158 |
| H    | 6.532  | 2.553 | 10.632 | Cu   | 5.170  | 6.625  | 6.153 | Cu   | 0.960  | 0.371  | 3.137 |
| H    | 6.147  | 3.535 | 9.194  | Cu   | 3.370  | 2.510  | 6.100 | Cu   | 2.686  | 6.901  | 2.493 |
| H    | 8.487  | 4.018 | 11.139 | Cu   | 8.796  | 6.640  | 5.508 | Cu   | 0.837  | 2.828  | 2.458 |
| H    | 7.597  | 6.072 | 10.208 | Cu   | 6.959  | 2.578  | 5.521 | Cu   | 8.230  | 8.450  | 2.467 |
| H    | 9.068  | 5.710 | 9.513  | Cu   | 3.260  | 5.092  | 5.551 | Cu   | 6.382  | 4.403  | 2.503 |
| N    | 8.085  | 5.421 | 9.587  | Cu   | 1.395  | 0.988  | 5.537 | Cu   | 11.863 | 8.472  | 1.918 |
| O    | 10.093 | 3.619 | 9.021  | Cu   | -0.549 | -0.583 | 4.948 | Cu   | 9.995  | 4.406  | 1.865 |
| O    | 8.376  | 2.179 | 8.642  | Cu   | 1.295  | 3.465  | 4.852 | Cu   | 6.304  | 6.908  | 1.888 |
|      |        |       |        | Cu   | 4.986  | 0.971  | 4.870 | Cu   | 4.477  | 2.846  | 1.878 |
|      |        |       |        | Cu   | 6.822  | 5.057  | 4.914 | Cu   | 9.899  | 6.905  | 1.342 |
|      |        |       |        | Cu   | 12.276 | 9.136  | 4.360 | Cu   | 8.047  | 2.850  | 1.335 |
| Au   | 7.260  | 5.634 | 7.403  | Cu   | 10.418 | 5.047  | 4.275 | Cu   | 4.360  | 5.347  | 1.360 |
| Au   | 1.707  | 4.011 | 7.375  | Cu   | 6.713  | 7.557  | 4.296 | Cu   | 2.511  | 1.284  | 1.342 |
| Cu   | 5.408  | 1.624 | 7.173  | Cu   | 4.869  | 3.493  | 4.302 | Cu   | 6.131  | 1.272  | 0.856 |
| Cu   | -0.076 | 0.103 | 7.294  | Cu   | 10.328 | 7.546  | 3.714 | Cu   | 7.939  | 5.338  | 0.851 |
| Cu   | 12.648 | 9.727 | 6.782  | Cu   | 8.470  | 3.485  | 3.700 | Cu   | 0.557  | -0.285 | 0.852 |
| Cu   | 10.785 | 5.668 | 6.632  | Cu   | 4.772  | 5.991  | 3.733 | Cu   | 2.423  | 3.792  | 0.867 |

**Table S68:** Coordinates for the most stable L-alanine adsorbed on Au-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.168  | 3.861 | 10.006 | Cu   | 7.284  | 8.301  | 6.728 | Cu   | 3.080  | 2.044  | 3.748 |
| C    | 7.667  | 2.640 | 9.206  | Cu   | 5.391  | 4.207  | 6.679 | Cu   | 8.497  | 6.136  | 3.188 |
| C    | 9.620  | 4.317 | 9.701  | Cu   | 10.851 | 8.244  | 6.160 | Cu   | 6.650  | 2.062  | 3.167 |
| H    | 10.036 | 4.826 | 10.587 | Cu   | 9.051  | 4.173  | 6.146 | Cu   | 2.969  | 4.571  | 3.191 |
| H    | 9.912  | 2.441 | 9.238  | Cu   | 5.320  | 6.733  | 6.169 | Cu   | 1.101  | 0.505  | 3.189 |
| H    | 9.578  | 5.044 | 8.868  | Cu   | 3.557  | 2.591  | 6.134 | Cu   | 2.818  | 7.033  | 2.534 |
| H    | 8.116  | 3.539 | 11.065 | Cu   | 8.927  | 6.731  | 5.588 | Cu   | 0.973  | 2.960  | 2.503 |
| H    | 7.412  | 5.759 | 10.418 | Cu   | 7.094  | 2.674  | 5.548 | Cu   | 8.379  | 8.599  | 2.530 |
| H    | 6.289  | 4.670 | 9.834  | Cu   | 3.413  | 5.196  | 5.577 | Cu   | 6.521  | 4.542  | 2.536 |
| N    | 7.259  | 4.996 | 9.753  | Cu   | 1.547  | 1.095  | 5.579 | Cu   | 11.985 | 8.608  | 1.956 |
| O    | 6.428  | 2.573 | 8.958  | Cu   | -0.420 | -0.469 | 4.983 | Cu   | 10.133 | 4.541  | 1.913 |
| O    | 12.234 | 9.873 | 8.894  | Cu   | 1.436  | 3.569  | 4.888 | Cu   | 6.451  | 7.056  | 1.928 |
| O    | -0.556 | 0.129 | 9.341  | Cu   | 5.158  | 1.092  | 4.970 | Cu   | 4.613  | 2.993  | 1.907 |
|      |        |       |        | Cu   | 6.979  | 5.163  | 4.943 | Cu   | 10.039 | 7.049  | 1.387 |
|      |        |       |        | Cu   | 12.406 | 9.238  | 4.376 | Cu   | 8.175  | 2.988  | 1.372 |
| Au   | 7.387  | 5.751 | 7.464  | Cu   | 10.543 | 5.159  | 4.328 | Cu   | 4.500  | 5.495  | 1.392 |
| Au   | 1.888  | 4.067 | 7.390  | Cu   | 6.865  | 7.684  | 4.339 | Cu   | 2.657  | 1.429  | 1.384 |
| Cu   | 5.599  | 1.714 | 7.314  | Cu   | 5.018  | 3.608  | 4.328 | Cu   | 6.250  | 1.412  | 0.881 |
| Cu   | 0.068  | 0.182 | 7.314  | Cu   | 10.454 | 7.662  | 3.769 | Cu   | 8.086  | 5.485  | 0.905 |
| Cu   | 12.783 | 9.804 | 6.775  | Cu   | 8.605  | 3.611  | 3.746 | Cu   | 0.699  | -0.142 | 0.902 |
| Cu   | 10.926 | 5.747 | 6.684  | Cu   | 4.917  | 6.119  | 3.767 | Cu   | 2.552  | 3.943  | 0.906 |

**Table S69:** Coordinates for the most stable D- $\mu_3$ -serine adsorbed on Au-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.585  | 4.511  | 10.096 | Cu   | 7.221  | 8.229  | 6.712 | Cu   | 3.009  | 1.954  | 3.792 |
| C    | 9.904  | 4.503  | 9.315  | Cu   | 5.321  | 4.105  | 6.738 | Cu   | 8.460  | 6.029  | 3.202 |
| C    | 7.782  | 3.234  | 9.751  | Cu   | 10.799 | 8.216  | 6.202 | Cu   | 6.599  | 1.989  | 3.208 |
| H    | 5.928  | 3.631  | 9.266  | Cu   | 9.016  | 4.111  | 6.154 | Cu   | 2.883  | 4.463  | 3.224 |
| H    | 8.204  | 2.386  | 10.306 | Cu   | 5.286  | 6.634  | 6.111 | Cu   | 1.055  | 0.404  | 3.206 |
| H    | 7.892  | 3.028  | 8.668  | Cu   | 3.435  | 2.549  | 6.184 | Cu   | 2.772  | 6.926  | 2.547 |
| H    | 8.793  | 4.532  | 11.181 | Cu   | 8.915  | 6.661  | 5.593 | Cu   | 0.918  | 2.863  | 2.557 |
| H    | 6.955  | 5.764  | 10.260 | Cu   | 7.042  | 2.614  | 5.606 | Cu   | 8.315  | 8.480  | 2.528 |
| H    | 8.378  | 6.547  | 9.828  | Cu   | 3.368  | 5.126  | 5.575 | Cu   | 6.476  | 4.435  | 2.547 |
| N    | 7.809  | 5.705  | 9.697  | Cu   | 1.471  | 1.024  | 5.619 | Cu   | 11.937 | 8.502  | 1.949 |
| O    | 10.287 | 5.605  | 8.812  | Cu   | -0.454 | -0.544 | 4.968 | Cu   | 10.097 | 4.446  | 1.973 |
| O    | -0.622 | 0.242  | 9.153  | Cu   | 1.355  | 3.485  | 4.977 | Cu   | 6.395  | 6.930  | 1.932 |
| O    | 6.401  | 3.364  | 10.086 | Cu   | 5.080  | 1.005  | 4.940 | Cu   | 4.549  | 2.878  | 1.942 |
|      |        |        |        | Cu   | 6.931  | 5.073  | 4.960 | Cu   | 9.994  | 6.938  | 1.406 |
|      |        |        |        | Cu   | 12.339 | 9.152  | 4.357 | Cu   | 8.143  | 2.889  | 1.405 |
| Au   | 7.291  | 5.674  | 7.444  | Cu   | 10.518 | 5.099  | 4.423 | Cu   | 4.433  | 5.370  | 1.406 |
| Au   | 1.872  | 4.192  | 7.461  | Cu   | 6.820  | 7.583  | 4.340 | Cu   | 2.587  | 1.317  | 1.421 |
| Cu   | 5.484  | 1.664  | 7.251  | Cu   | 4.955  | 3.524  | 4.353 | Cu   | 6.204  | 1.312  | 0.925 |
| Cu   | 0.027  | -0.087 | 7.327  | Cu   | 10.412 | 7.582  | 3.787 | Cu   | 8.057  | 5.372  | 0.916 |
| Cu   | 12.734 | 9.794  | 6.727  | Cu   | 8.567  | 3.524  | 3.778 | Cu   | 0.641  | -0.244 | 0.917 |
| Cu   | 10.927 | 5.689  | 6.871  | Cu   | 4.866  | 6.006  | 3.750 | Cu   | 2.487  | 3.801  | 0.934 |

**Table S70:** Coordinates for the most stable L- $\mu_3$ -serine adsorbed on Au-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 5.453  | 5.001  | 9.943  | Cu   | 7.459  | 8.098 | 6.653 | Cu   | 3.201  | 1.842 | 3.726 |
| C    | 4.239  | 5.656  | 9.239  | Cu   | 5.498  | 4.046 | 6.709 | Cu   | 8.633  | 5.917 | 3.149 |
| C    | 5.563  | 3.485  | 9.719  | Cu   | 10.934 | 8.062 | 6.153 | Cu   | 6.774  | 1.863 | 3.131 |
| H    | 4.589  | 3.060  | 10.024 | Cu   | 9.213  | 3.978 | 6.144 | Cu   | 3.077  | 4.347 | 3.146 |
| H    | 6.341  | 3.096  | 10.409 | Cu   | 5.501  | 6.514 | 6.064 | Cu   | 1.246  | 0.300 | 3.153 |
| H    | 5.242  | 5.120  | 11.026 | Cu   | 3.624  | 2.410 | 6.093 | Cu   | 2.959  | 6.811 | 2.492 |
| H    | 7.430  | 5.522  | 10.291 | Cu   | 9.075  | 6.494 | 5.544 | Cu   | 1.121  | 2.766 | 2.509 |
| H    | 6.487  | 6.736  | 9.643  | Cu   | 7.222  | 2.475 | 5.495 | Cu   | 8.504  | 8.382 | 2.484 |
| N    | 6.700  | 5.732  | 9.605  | Cu   | 3.550  | 5.005 | 5.495 | Cu   | 6.654  | 4.321 | 2.487 |
| O    | 4.415  | 6.872  | 8.865  | Cu   | 1.671  | 0.874 | 5.576 | Cu   | 12.115 | 8.398 | 1.891 |
| O    | 3.180  | 4.980  | 9.175  | Cu   | 3.414  | 7.456 | 4.913 | Cu   | 10.290 | 4.333 | 1.888 |
| O    | 5.907  | 3.122  | 8.407  | Cu   | 1.549  | 3.376 | 4.920 | Cu   | 6.586  | 6.829 | 1.877 |
|      |        |        |        | Cu   | 8.976  | 9.013 | 4.915 | Cu   | 4.728  | 2.782 | 1.897 |
|      |        |        |        | Cu   | 7.120  | 4.936 | 4.917 | Cu   | 10.177 | 6.838 | 1.357 |
|      |        |        |        | Cu   | 12.520 | 9.017 | 4.304 | Cu   | 8.330  | 2.774 | 1.345 |
| Au   | 7.595  | 5.575  | 7.446  | Cu   | 10.692 | 4.955 | 4.310 | Cu   | 4.621  | 5.265 | 1.345 |
| Au   | 1.985  | 4.006  | 7.373  | Cu   | 7.005  | 7.466 | 4.286 | Cu   | 2.775  | 1.218 | 1.356 |
| Cu   | 5.691  | 1.534  | 7.271  | Cu   | 5.153  | 3.422 | 4.328 | Cu   | 10.066 | 9.340 | 0.853 |
| Cu   | 0.120  | -0.208 | 7.303  | Cu   | 10.581 | 7.458 | 3.735 | Cu   | 8.230  | 5.260 | 0.868 |
| Cu   | 12.880 | 9.651  | 6.656  | Cu   | 8.746  | 3.406 | 3.712 | Cu   | 4.530  | 7.743 | 0.866 |
| Cu   | 11.101 | 5.494  | 6.719  | Cu   | 5.057  | 5.900 | 3.707 | Cu   | 2.679  | 3.711 | 0.855 |

**Table S71:** Coordinates for the most stable D- $\mu_4$ -serine adsorbed on Au-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 6.850  | 7.609  | 10.010 | Cu   | 7.418  | 7.981 | 6.776 | Cu   | 3.212  | 1.702 | 3.773 |
| C    | 2.005  | 0.260  | 9.312  | Cu   | 5.558  | 3.874 | 6.725 | Cu   | 8.631  | 5.786 | 3.206 |
| C    | 8.208  | 8.255  | 9.744  | Cu   | 10.989 | 7.911 | 6.173 | Cu   | 6.785  | 1.729 | 3.182 |
| H    | 4.449  | 1.174  | 10.125 | Cu   | 9.147  | 3.851 | 6.209 | Cu   | 3.089  | 4.230 | 3.232 |
| H    | 8.979  | 7.713  | 10.330 | Cu   | 5.465  | 6.406 | 6.162 | Cu   | 1.233  | 0.155 | 3.203 |
| H    | 6.657  | 7.716  | 11.096 | Cu   | 3.683  | 2.309 | 6.143 | Cu   | 2.961  | 6.689 | 2.547 |
| H    | 7.285  | 5.609  | 10.366 | Cu   | 9.080  | 6.376 | 5.593 | Cu   | 1.108  | 2.612 | 2.549 |
| H    | 5.822  | 5.892  | 9.611  | Cu   | 7.202  | 2.334 | 5.580 | Cu   | 8.496  | 8.233 | 2.520 |
| N    | 6.813  | 6.166  | 9.648  | Cu   | 3.553  | 4.875 | 5.619 | Cu   | 6.658  | 4.203 | 2.575 |
| O    | 4.710  | 7.612  | 8.953  | Cu   | 1.691  | 0.767 | 5.593 | Cu   | 12.121 | 8.257 | 1.941 |
| O    | 2.089  | 1.494  | 9.189  | Cu   | 3.380  | 7.321 | 4.975 | Cu   | 10.265 | 4.203 | 1.955 |
| O    | 8.574  | 8.227  | 8.383  | Cu   | 1.560  | 3.227 | 4.944 | Cu   | 6.566  | 6.708 | 1.977 |
|      |        |        |        | Cu   | 8.979  | 8.863 | 4.938 | Cu   | 4.748  | 2.638 | 1.944 |
|      |        |        |        | Cu   | 7.129  | 4.837 | 4.992 | Cu   | 10.174 | 6.692 | 1.402 |
|      |        |        |        | Cu   | 12.519 | 8.891 | 4.351 | Cu   | 8.316  | 2.648 | 1.397 |
| Au   | 7.537  | 5.416  | 7.527  | Cu   | 10.684 | 4.810 | 4.390 | Cu   | 4.632  | 5.148 | 1.432 |
| Au   | 2.010  | 3.843  | 7.441  | Cu   | 7.013  | 7.353 | 4.403 | Cu   | 2.780  | 1.076 | 1.403 |
| Cu   | 5.785  | 1.447  | 7.311  | Cu   | 5.155  | 3.275 | 4.359 | Cu   | 10.067 | 9.172 | 0.904 |
| Cu   | 0.067  | -0.233 | 7.305  | Cu   | 10.589 | 7.314 | 3.781 | Cu   | 8.209  | 5.153 | 0.924 |
| Cu   | 12.878 | 9.501  | 6.745  | Cu   | 8.731  | 3.274 | 3.774 | Cu   | 4.528  | 7.636 | 0.907 |
| Cu   | 11.076 | 5.386  | 6.768  | Cu   | 5.051  | 5.776 | 3.806 | Cu   | 2.694  | 3.569 | 0.945 |

**Table S72:** Coordinates for the most stable L- $\mu_4$ -serine adsorbed on Au-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y     | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|-------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.102  | 3.919 | 10.007 | Cu   | 7.278  | 8.315  | 6.719 | Cu   | 3.092  | 2.032  | 3.731 |
| C    | 7.639  | 2.688 | 9.188  | Cu   | 5.385  | 4.217  | 6.670 | Cu   | 8.510  | 6.106  | 3.186 |
| C    | 9.511  | 4.492 | 9.748  | Cu   | 10.857 | 8.262  | 6.155 | Cu   | 6.665  | 2.033  | 3.174 |
| H    | 9.764  | 5.181 | 10.569 | Cu   | 9.064  | 4.188  | 6.145 | Cu   | 2.982  | 4.548  | 3.186 |
| H    | 2.624  | 7.244 | 9.397  | Cu   | 5.324  | 6.739  | 6.143 | Cu   | 1.118  | 0.477  | 3.175 |
| H    | 9.483  | 5.072 | 8.810  | Cu   | 3.550  | 2.605  | 6.122 | Cu   | 2.837  | 6.998  | 2.533 |
| H    | 8.046  | 3.591 | 11.065 | Cu   | 8.932  | 6.735  | 5.584 | Cu   | 0.987  | 2.924  | 2.498 |
| H    | 7.263  | 5.790 | 10.402 | Cu   | 7.103  | 2.680  | 5.550 | Cu   | 8.394  | 8.563  | 2.529 |
| H    | 6.194  | 4.659 | 9.784  | Cu   | 3.415  | 5.205  | 5.566 | Cu   | 6.537  | 4.503  | 2.532 |
| N    | 7.152  | 5.020 | 9.737  | Cu   | 1.561  | 1.107  | 5.546 | Cu   | 12.005 | 8.564  | 1.959 |
| O    | 6.397  | 2.611 | 8.941  | Cu   | -0.408 | -0.464 | 4.981 | Cu   | 10.151 | 4.497  | 1.913 |
| O    | 12.199 | 9.924 | 8.867  | Cu   | 1.446  | 3.571  | 4.878 | Cu   | 6.472  | 7.012  | 1.923 |
| S    | -0.172 | 0.182 | 9.595  | Cu   | 5.160  | 1.090  | 4.965 | Cu   | 4.638  | 2.951  | 1.902 |
|      |        |       |        | Cu   | 6.987  | 5.151  | 4.932 | Cu   | 10.047 | 7.004  | 1.388 |
|      |        |       |        | Cu   | 12.417 | 9.233  | 4.380 | Cu   | 8.195  | 2.939  | 1.379 |
| Au   | 7.373  | 5.770 | 7.444  | Cu   | 10.559 | 5.147  | 4.324 | Cu   | 4.520  | 5.451  | 1.387 |
| Au   | 1.890  | 4.091 | 7.383  | Cu   | 6.877  | 7.669  | 4.330 | Cu   | 2.677  | 1.382  | 1.376 |
| Cu   | 5.589  | 1.725 | 7.307  | Cu   | 5.029  | 3.595  | 4.325 | Cu   | 6.273  | 1.365  | 0.887 |
| Cu   | 0.117  | 0.204 | 7.316  | Cu   | 10.464 | 7.643  | 3.770 | Cu   | 8.104  | 5.431  | 0.904 |
| Cu   | 12.800 | 9.831 | 6.787  | Cu   | 8.621  | 3.591  | 3.748 | Cu   | 0.719  | -0.188 | 0.897 |
| Cu   | 10.939 | 5.763 | 6.670  | Cu   | 4.931  | 6.098  | 3.755 | Cu   | 2.576  | 3.892  | 0.907 |

**Table S73:** Coordinates for the most stable D- $\mu_3$ -cysteine adsorbed on Au-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.480  | 4.213  | 10.033 | Cu   | 7.235  | 8.304  | 6.773 | Cu   | 3.028  | 2.020  | 3.832 |
| C    | 9.878  | 4.376  | 9.376  | Cu   | 5.333  | 4.195  | 6.698 | Cu   | 8.480  | 6.089  | 3.243 |
| C    | 7.845  | 2.983  | 9.359  | Cu   | 10.806 | 8.270  | 6.257 | Cu   | 6.610  | 2.032  | 3.230 |
| H    | 5.659  | 3.905  | 9.052  | Cu   | 9.034  | 4.167  | 6.170 | Cu   | 2.900  | 4.519  | 3.247 |
| H    | 8.342  | 2.066  | 9.704  | Cu   | 5.308  | 6.702  | 6.128 | Cu   | 1.084  | 0.471  | 3.251 |
| H    | 7.998  | 3.060  | 8.266  | Cu   | 3.466  | 2.611  | 6.223 | Cu   | 2.793  | 6.972  | 2.568 |
| H    | 8.599  | 4.036  | 11.117 | Cu   | 8.926  | 6.728  | 5.640 | Cu   | 0.932  | 2.924  | 2.590 |
| H    | 6.866  | 5.495  | 10.345 | Cu   | 7.056  | 2.659  | 5.621 | Cu   | 8.346  | 8.562  | 2.610 |
| H    | 8.307  | 6.257  | 9.964  | Cu   | 3.374  | 5.180  | 5.587 | Cu   | 6.498  | 4.484  | 2.571 |
| N    | 7.711  | 5.444  | 9.770  | Cu   | 1.483  | 1.099  | 5.674 | Cu   | 11.942 | 8.550  | 1.970 |
| O    | 10.198 | 5.527  | 8.955  | Cu   | -0.430 | -0.484 | 4.983 | Cu   | 10.122 | 4.498  | 2.015 |
| O    | -0.539 | 0.174  | 9.223  | Cu   | 1.365  | 3.547  | 5.013 | Cu   | 6.437  | 6.992  | 1.972 |
| S    | 6.051  | 2.697  | 9.566  | Cu   | 5.113  | 1.095  | 5.052 | Cu   | 4.573  | 2.942  | 1.966 |
|      |        |        |        | Cu   | 6.957  | 5.128  | 4.969 | Cu   | 9.994  | 6.996  | 1.449 |
|      |        |        |        | Cu   | 12.348 | 9.201  | 4.371 | Cu   | 8.160  | 2.928  | 1.433 |
| Au   | 7.301  | 5.744  | 7.460  | Cu   | 10.533 | 5.162  | 4.471 | Cu   | 4.467  | 5.427  | 1.429 |
| Au   | 1.875  | 4.228  | 7.490  | Cu   | 6.843  | 7.660  | 4.386 | Cu   | 2.625  | 1.378  | 1.459 |
| Cu   | 5.535  | 1.746  | 7.417  | Cu   | 4.972  | 3.570  | 4.370 | Cu   | 6.203  | 1.364  | 0.947 |
| Cu   | 0.046  | -0.048 | 7.348  | Cu   | 10.417 | 7.644  | 3.831 | Cu   | 8.082  | 5.409  | 0.954 |
| Cu   | 12.774 | 9.825  | 6.713  | Cu   | 8.585  | 3.571  | 3.798 | Cu   | 0.676  | -0.183 | 0.964 |
| Cu   | 10.902 | 5.747  | 6.957  | Cu   | 4.888  | 6.064  | 3.770 | Cu   | 2.513  | 3.863  | 0.965 |

**Table S74:** Coordinates for the most stable L- $\mu_3$ -cysteine adsorbed on Au-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y     | z     | Atom | x      | y     | z     |
|------|--------|--------|--------|------|--------|-------|-------|------|--------|-------|-------|
| C    | 9.074  | 5.731  | 9.921  | Cu   | 7.177  | 7.946 | 7.001 | Cu   | 2.988  | 1.713 | 3.808 |
| C    | 9.805  | 4.419  | 9.492  | Cu   | 5.225  | 3.844 | 6.747 | Cu   | 8.406  | 5.793 | 3.248 |
| C    | 9.514  | 6.990  | 9.167  | Cu   | 10.797 | 7.982 | 6.193 | Cu   | 6.557  | 1.739 | 3.251 |
| H    | 10.433 | 7.393  | 9.615  | Cu   | 8.978  | 3.873 | 6.161 | Cu   | 2.862  | 4.242 | 3.252 |
| H    | 9.754  | 6.714  | 8.124  | Cu   | 5.219  | 6.413 | 6.228 | Cu   | 1.031  | 0.173 | 3.243 |
| H    | 9.263  | 5.860  | 11.002 | Cu   | 3.400  | 2.277 | 6.206 | Cu   | 2.750  | 6.705 | 2.588 |
| H    | 7.053  | 6.181  | 10.096 | Cu   | 8.864  | 6.405 | 5.635 | Cu   | 0.887  | 2.624 | 2.562 |
| H    | 7.425  | 4.537  | 10.150 | Cu   | 6.979  | 2.358 | 5.652 | Cu   | 8.279  | 8.252 | 2.606 |
| N    | 7.637  | 5.436  | 9.701  | Cu   | 3.316  | 4.903 | 5.602 | Cu   | 6.438  | 4.197 | 2.598 |
| O    | 9.330  | 3.350  | 9.897  | Cu   | 1.495  | 0.767 | 5.634 | Cu   | 11.896 | 8.267 | 1.994 |
| O    | 10.847 | 4.515  | 8.704  | Cu   | 3.208  | 7.342 | 5.024 | Cu   | 10.047 | 4.213 | 1.993 |
| S    | 8.281  | 8.361  | 9.030  | Cu   | 1.336  | 3.240 | 4.972 | Cu   | 6.368  | 6.719 | 2.030 |
|      |        |        |        | Cu   | 8.735  | 8.883 | 5.036 | Cu   | 4.525  | 2.654 | 1.978 |
|      |        |        |        | Cu   | 6.875  | 4.834 | 4.992 | Cu   | 9.933  | 6.703 | 1.453 |
|      |        |        |        | Cu   | 12.313 | 8.930 | 4.398 | Cu   | 8.093  | 2.647 | 1.446 |
| Au   | 7.225  | 5.271  | 7.468  | Cu   | 10.487 | 4.849 | 4.423 | Cu   | 4.423  | 5.160 | 1.457 |
| Au   | 1.838  | 3.945  | 7.468  | Cu   | 6.804  | 7.364 | 4.496 | Cu   | 2.580  | 1.090 | 1.437 |
| Cu   | 5.512  | 1.442  | 7.388  | Cu   | 4.911  | 3.269 | 4.394 | Cu   | 9.840  | 9.180 | 0.966 |
| Cu   | -0.032 | -0.174 | 7.375  | Cu   | 10.366 | 7.340 | 3.826 | Cu   | 7.992  | 5.148 | 0.955 |
| Cu   | 12.711 | 9.591  | 6.808  | Cu   | 8.520  | 3.284 | 3.806 | Cu   | 4.324  | 7.655 | 0.957 |
| Cu   | 10.915 | 5.456  | 6.812  | Cu   | 4.838  | 5.790 | 3.821 | Cu   | 2.472  | 3.586 | 0.966 |

**Table S75:** Coordinates for the most stable D- $\mu_4$ -cysteine adsorbed on Au-50%-decorated Cu(531)<sup>S</sup>.

| Atom | x      | y      | z      | Atom | x      | y      | z     | Atom | x      | y      | z     |
|------|--------|--------|--------|------|--------|--------|-------|------|--------|--------|-------|
| C    | 8.365  | 4.232  | 9.947  | Cu   | 7.239  | 8.317  | 6.740 | Cu   | 3.064  | 2.012  | 3.859 |
| C    | 9.785  | 4.343  | 9.340  | Cu   | 5.399  | 4.138  | 7.014 | Cu   | 8.501  | 6.076  | 3.253 |
| C    | 7.655  | 3.037  | 9.250  | Cu   | 10.845 | 8.250  | 6.239 | Cu   | 6.645  | 2.035  | 3.257 |
| H    | 7.932  | 2.111  | 9.768  | Cu   | 9.059  | 4.154  | 6.179 | Cu   | 2.946  | 4.511  | 3.294 |
| H    | 8.044  | 2.965  | 8.214  | Cu   | 5.346  | 6.668  | 6.154 | Cu   | 1.112  | 0.465  | 3.264 |
| H    | 8.448  | 4.023  | 11.029 | Cu   | 3.491  | 2.610  | 6.228 | Cu   | 2.829  | 6.969  | 2.589 |
| H    | 6.734  | 5.492  | 10.163 | Cu   | 8.965  | 6.730  | 5.620 | Cu   | 0.975  | 2.920  | 2.614 |
| H    | 8.214  | 6.288  | 10.071 | Cu   | 7.086  | 2.641  | 5.640 | Cu   | 8.375  | 8.540  | 2.602 |
| N    | 7.657  | 5.505  | 9.716  | Cu   | 3.464  | 5.151  | 5.661 | Cu   | 6.526  | 4.481  | 2.604 |
| O    | 10.171 | 5.481  | 8.932  | Cu   | 1.490  | 1.082  | 5.689 | Cu   | 11.981 | 8.553  | 1.998 |
| O    | -0.664 | 0.119  | 9.199  | Cu   | -0.396 | -0.504 | 5.010 | Cu   | 10.151 | 4.493  | 2.026 |
| S    | 5.823  | 3.095  | 9.076  | Cu   | 1.392  | 3.531  | 5.036 | Cu   | 6.457  | 6.983  | 1.979 |
|      |        |        |        | Cu   | 5.139  | 1.076  | 5.025 | Cu   | 4.603  | 2.942  | 2.045 |
|      |        |        |        | Cu   | 6.975  | 5.106  | 5.019 | Cu   | 10.034 | 6.991  | 1.457 |
|      |        |        |        | Cu   | 12.399 | 9.189  | 4.403 | Cu   | 8.193  | 2.932  | 1.454 |
| Au   | 7.404  | 5.838  | 7.460  | Cu   | 10.563 | 5.152  | 4.477 | Cu   | 4.495  | 5.422  | 1.452 |
| Au   | 1.890  | 4.206  | 7.503  | Cu   | 6.865  | 7.635  | 4.382 | Cu   | 2.657  | 1.374  | 1.482 |
| Cu   | 5.526  | 1.629  | 7.388  | Cu   | 5.037  | 3.595  | 4.495 | Cu   | 6.231  | 1.380  | 0.971 |
| Cu   | 0.090  | -0.079 | 7.389  | Cu   | 10.458 | 7.638  | 3.825 | Cu   | 8.104  | 5.407  | 0.968 |
| Cu   | 12.807 | 9.811  | 6.746  | Cu   | 8.617  | 3.563  | 3.820 | Cu   | 0.705  | -0.191 | 0.972 |
| Cu   | 10.917 | 5.716  | 6.983  | Cu   | 4.920  | 6.054  | 3.794 | Cu   | 2.561  | 3.862  | 1.003 |

**Table S76:** Coordinates for the most stable L- $\mu_4$ -cysteine adsorbed on Au-50%-decorated Cu(531)<sup>S</sup>.