Supporting Information for "Ab Initio DFT+U Analysis of Oxygen Vacancy Formation and Migration in $La_{1-x}Sr_xFeO_{3-\delta}$ (x=0, 0.25 and 0.50)"

Andrew M. Ritzmann, Michele Pavone, Ana B. Muñoz-García, John A. Keith and Emily A. Carter

[1]Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ 08544-5263, United States, [2]Department of Chemical Sciences, University of Naples Federico II, Naples 80126, Italy [3]Department of Mechanical and Aerospace Engineering, [4]Program in Applied and Computational Mathematics, and Andlinger Center for Energy and the Environment, Princeton University, Princeton, New Jersey 08544-5263, United States

Thermal Contributions from the O_2 Molecule

Our work presents oxygen vacancy enthalpies and free energies in $La_{1-x}Sr_xFeO_3$. While the thermal contributions from the solids are clearly defined in the text, the thermal contributions from the O_2 molecule are compressed into terms related to the enthalpy ($\int_0^T C_{p,O_2}(T')dT'$, equation 5) and the entropy ($S_{O_2}(T)$, equation 7). We compute these from the standard ideal gas, rigid-rotor, and harmonic oscillator approximations.[S1] We also take into account the

degeneracy of the electronic ground state (triplet O_2). Equation S1 gives the enthalpy contribution (excluding the zero-point energy, which was already accounted for in equation 4 of the main text).

$$H(T) - H(0\,\mathrm{K}) = \int_0^T C_\mathrm{P}(T')dT' = k_\mathrm{B}T\left(\frac{7}{2} + \frac{\Theta_v}{T}\frac{1}{e^{\frac{\Theta_v}{T}} - 1}\right) \tag{S1}$$

In equation S1, H is the enthalpy, R is the gas constant, T is the absolute temperature and Θ_v is the vibrational temperature. The factor of 7/2 arises from the ideal gas and rigid-rotor approximations for a homonuclear diatomic molecule. Θ_v is defined in equation S2 where ν is the vibrational frequency, h is Planck's constant and k_B is Boltzmann's constant.

$$\Theta_v = \frac{h\nu}{k_B} \tag{S2}$$

The entropy is defined in equation S3 where the unimolecular partition functions for translation (q_t), rotation (q_r), vibration (q_v) and electronic motion (q_e) are defined in equations S4-S7.

$$s = s_e + s_t + s_r + s_v = k_\mathrm{B}\left(\ln(q_e) + \left[\ln(q_t) + \frac{5}{2}\right] + \left[\ln(q_v) + \frac{\Theta_v}{T}\frac{1}{e^{\frac{\Theta_v}{T}} - 1}\right] + \left[\ln(q_r) + 1\right]\right) \tag{S3}$$

$$q_\mathrm{t} = \left(\frac{2\pi M\, k_\mathrm{B}T}{h^2}\right)^{3/2} V \tag{S4}$$

$$q_\mathrm{r} = \left(\frac{8\pi^2\, I\, k_\mathrm{B}T}{2h^2}\right) \tag{S5}$$

$$q_\mathrm{v} = \left(\frac{1}{1 - e^{\frac{-h\nu}{k_\mathrm{B}T}}}\right) \tag{S6}$$

$$q_e = 3 \quad \text{(triplet ground state)} \tag{S7}$$

In equations S4-S7, M is the mass of the molecule, I is the moment of inertia, and V is the volume per molecule (eventually equated to RT/P through the ideal gas approximation).

In order to use these equations to calculate the thermal corrections for the O_2 molecule, two quantities, the vibrational frequency (ν) and the equilibrium bond length (r_e) are required. For reference, we report the ν, r_e and D_0 (bond dissociation energy) values obtained for an O_2 molecule in a large box (9.0 × 9.1 × 9.2 Å) with DFT-GGA (computed with the Vienna ab Initio Simulation Package using the same projector-augmented wave potential described in the text and an elevated kinetic energy cutoff of 900 eV) and compare them to the experimental values (table S1). To validate our thermal corrections against reference data, we plot the enthalpy (figure S1) and entropy (figure S2) against the values obtained from the NIST webbook.[S2] The results show that DFT-GGA gives accurate values for the equilibrium bond length and vibrational frequency in O2. This leads to accurate calculation of the thermal corrections, namely the enthalpy (H) and entropy (S). The overestimation of the bond dissociation energy (D_0) for O_2 by DFT-GGA is well known and consistent with our results.

Table S1. DFT-GGA and experimental vibrational frequencies (ν), equilibrium bond lengths (r_e) and bond dissociation energies (D_0) for the O_2 molecule.

Quantity	DFT-PBE Results	Experiment
ν / cm^{-1}	1571	1580.19 [S3]
r_e / Å	1.232	1.20752 [S3]
D_0 / eV	5.96	5.12 [S4]

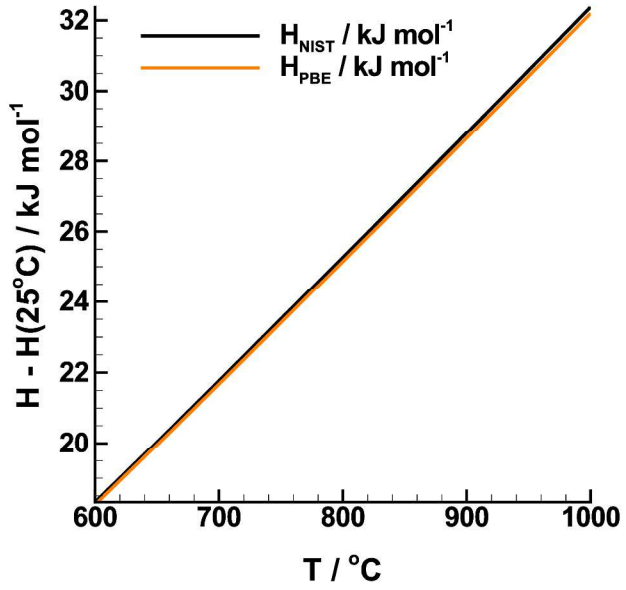

Figure S1. Enthalpy of the O_2 molecule (relative to 25°C) from the NIST webbook[S5] data (black) and computed using the parameters obtained from DFT-PBE (orange).

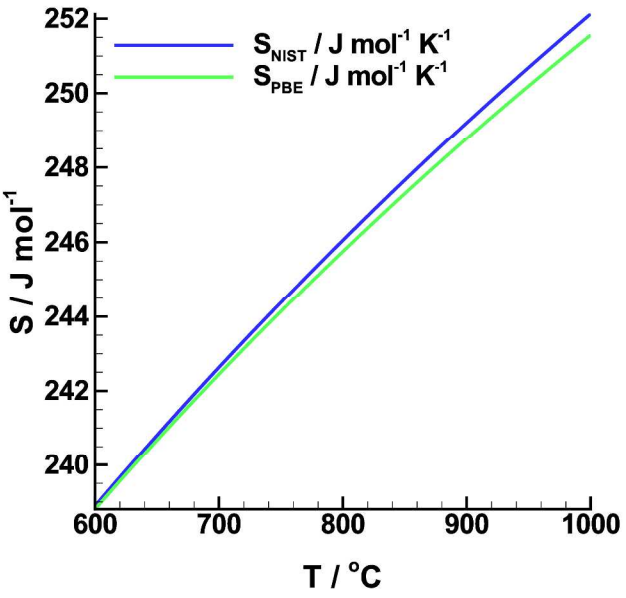

Figure S2. Entropy of the O_2 molecule from the NIST webbook[S5] data (blue) and computed using the parameters obtained from DFT-PBE (green).

Oxygen Vacancy Formation Free Energies as a Function of Temperature

Using the relationships described in the main text as well as the thermal corrections for O_2 (*vide supra*), we calculate the oxygen vacancy formation free energy ($\Delta G_{f,vac}$) as a function of temperature over the range 500-1000°C. As explained in the main text, we include all vibrational contributions from the crystal, but phonon dispersion is ignored because it leads to unphysical results in the 40-atom supercell (the computational cost of calculating the phonon spectrum for the 160-atom supercell is prohibitively high). For the purpose of comparison, we also plot the $\Delta G_{f,vac}$ using $\Delta H^0_{f,vac}$ and $\Delta S^0_{f,vac}$ determined from the experiments of Ishigaki *et al*.[S5]

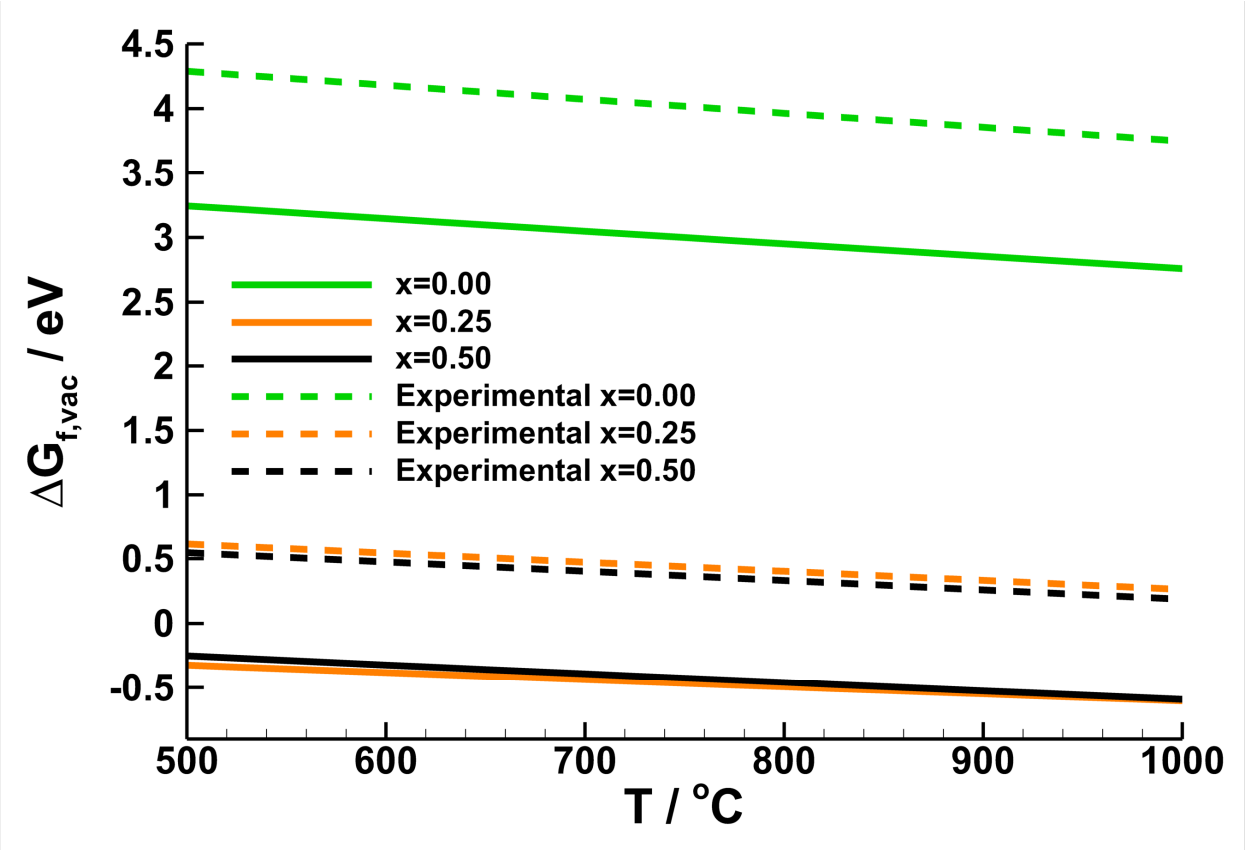

Figure S3. Free energies of oxygen vacancy formation for $LaFeO_3$ (green, x=0), $La_{0.75}Sr_{0.25}FeO_3$ (orange, x=0.25), and $La_{0.50}Sr_{0.50}FeO_3$ (black, x=0.50). The dashed lines provide the experimental data from reference S5 (assuming that $\Delta G_{f,vac} = \Delta H^0_{f,vac} - T\Delta S^0_{f,vac}$ and the standard enthalpies and entropies are independent of temperature).

We note that the computed values fall significantly below the experimental values, but this observation is consistent with what we see in the main text. Applying a correction for the overbinding of O_2 would shift the calculated lines upward by approximately 0.42 eV and yield significantly better agreement with experiment. The fact that the slopes of the calculated and experimental data are similar indicates that the entropy of vacancy formation does not have a strong temperature dependence. Finally, the ordering of x=0.25 and x=0.50 vacancy formation free energies is reversed in the calculated data compared with experiment; however, the difference between these two lines is very small, such that the two are essentially equal in both the experimental results and the computed results.

References

S1. McQuarrie, D. A.; Simon, J. D. Physical Chemistry: A Molecular Approach; 1st ed.; University Science Books: Sausalito, CA, 1997.

S2. Chase, M. W., Jr., *NIST-JANAF Thermochemical Tables*, 4th Edition, *J. Phys. Chem. Ref. Data, Monograph 9*, 1998, 1-1951

S3. "Spectroscopic Constants of Diatomic Molecules," in *CRC Handbook of Chemistry and Physics,* 93rd Edition, (Internet Version 2013), W. M. Haynes ed., CRC Press/Taylor and Francis, Boca Raton, FL.

S4. Darwent, B. deB., *Bond Dissociation Energies in Simple Molecules*, NSRDS-NBS-31, 1970

S5. Mizusaki, J.; Yoshihiro, M.; Yamauchi, S.; Fueki, K. *J. Solid State Chem.* 1985, *58*, 257–266.

Coordinates and Energies:

We report the optimized crystal structures for the pseudocubic cell and the sqs (160-atom) cell for x=0, 0.25, and 0.50. The information is given in the following format:
Description (Energy)
Lattice_vector_1-x Lattice_vector_1-y Lattice-vector_1_z
Lattice-vector_2-x Lattice-vector_2-y Lattice-vector_2-z
Lattice-vector_3-x Lattice-vector_3-y Lattice-vector_3-z
element_type fractional_coordinate-1 fractional_coordinate-2 fractional_coordinate-3

$LaFeO_3$ Pseudocubic Cell (-308.178 eV)
7.9107222177769509 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.9107222177769509 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.9107222177769509
Fe 0.7500032813284037 0.2499919425136596 0.0000121688575589
Fe 0.2499927822843944 0.7500094212620567 0.9999846441879967
Fe 0.2499992750903104 0.2499935302353435 0.9999945847173350
Fe 0.7500044874204264 0.7500061381813978 0.0000056489201299
Fe 0.7499946988057502 0.2499991287875218 0.4999882486674210
Fe 0.2500010876976120 0.7500022057223532 0.5000144657245329
Fe 0.2500078472524123 0.2499996634678681 0.5000027952303654
Fe 0.7499964043019816 0.7500001179375033 0.4999969581577091
La 0.4786038048858146 0.5138636508850780 0.2500111341905225
La 0.9785681257015924 0.0138934890632072 0.2499928566620753
La 0.5214073517981817 0.4861098063385825 0.7499890638395570
La 0.0214221687341336 0.9861177599952313 0.7500073643129781
La 0.0138393004002921 0.4786021677490311 0.7499983251689883
La 0.5138285096208861 0.9786054193521849 0.7499979788112512
La 0.9861454119079838 0.5213870909309364 0.2500017861473012
La 0.4861872379468153 0.0214163076307514 0.2500017820909335
O 0.7992597570088193 0.2807929938970659 0.2499988615650750
O 0.2992470294597425 0.7807840940647921 0.2499983766439087
O 0.2007477423679234 0.7192101408687535 0.7500012528384730
O 0.7007481096988073 0.2192124828479152 0.7500015402499258
O 0.2808104981619337 0.2992128894549992 0.7500014465751690
O 0.7808114868655665 0.7992054849496952 0.7500005355585202
O 0.7191867131624292 0.7007896638766269 0.2499972280942160
O 0.2191875152413445 0.2007922457052018 0.2500008103362390
O 0.2136018628890852 0.5004650554051793 0.0427490533516561
O 0.7135972334770031 0.0004539580918319 0.0427433749685306
O 0.7864000819569057 0.4995457849139626 0.9572503870822544
O 0.2864009407719195 0.9995345482949887 0.9572582133634100
O 0.0004416051950642 0.2135768933727036 0.9572929758496969
O 0.5004366413084824 0.7135732348672903 0.9572996992553939
O 0.9995663542068840 0.7864207384348987 0.0427059208180083
O 0.4995548111080126 0.2864308358037704 0.0427036743113902
O 0.7864041068402017 0.4995449426811973 0.5427513044517696

O 0.2863976660369332 0.9995362437118729 0.5427414643225390
O 0.2135981938994220 0.5004643480964219 0.4572494233508309
O 0.7136000708827837 0.0004538610354530 0.4572566596368404
O 0.9995669815755974 0.7864229701053205 0.4572948422733987
O 0.4995533607594638 0.2864290768549367 0.4572942951296710
O 0.0004423495302674 0.2135749623459091 0.5427061349739688
O 0.5004368424184023 0.7135746212664884 0.5427026913124635

$La_{0.75}Sr_{0.25}FeO_3$ Pseudocubic Cell (-295.099 eV)

7.8855807505787396 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.8855807505787396 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.8855807505787396
Fe 0.7500000452918840 0.2499994260168350 0.0000005634729447
Fe 0.2499996698446552 0.7500005862225194 0.9999997470918984
Fe 0.2500002800457963 0.2500002753997137 0.0000000499687332
Fe 0.7499994611023695 0.7499991964997079 0.0000000814329226
Fe 0.7499999958507289 0.2499994619745252 0.4999995159524673
Fe 0.2499996232159063 0.7500004853578730 0.5000003439091145
Fe 0.2500004745434694 0.2500002275075559 0.5000004029107856
Fe 0.7499991133572834 0.7499992981848180 0.4999998832512844
La 0.4856510933553011 0.5104968048876799 0.2503985798010078
La 0.9806340761293626 0.0136788302627338 0.2499778324362580
La 0.5193672710776980 0.4863245176329514 0.7500225029784957
La 0.0143426996383482 0.9895038823143310 0.7496013812705442
La 0.5068461638558972 0.9820945930371181 0.7492213897930284
La 0.9931551962149925 0.5179020289489955 0.2507789180335322
Sr 0.0124656053346968 0.4842317834685588 0.7504567702320202
Sr 0.4875360022123374 0.0157675641548209 0.2495432344176010
O 0.7952046210445118 0.2808091552737437 0.2490811185611150
O 0.2897808086298355 0.7659458089228721 0.2472016608451852
O 0.2102162163882042 0.7340566535172570 0.7527983605775788
O 0.7047977549190847 0.2191884367740258 0.7509186815003019
O 0.2877700156281406 0.2850854381037564 0.7529495631455632
O 0.7772161683311367 0.7928168457087921 0.7498401554249341
O 0.7227810061465050 0.7071801286201875 0.2501596942822815
O 0.2122325178342308 0.2149168663118530 0.2470504312739266
O 0.2211075082941392 0.4982138430586645 0.0380479909292291
O 0.7280391060293994 0.0037836757447778 0.0335582923340354
O 0.7719620607944435 0.4962156827501119 0.9664404673907683
O 0.2788930372643463 0.0017872016580327 0.9619514914759790
O 0.0030179458927719 0.2143213086815408 0.9633434829472520
O 0.4991104015590366 0.7216150453430927 0.9586043225777061
O 0.0008885514695578 0.7783851859104303 0.0413968232287516
O 0.4969834136909768 0.2856788954843807 0.0366562076051622
O 0.7733820901455246 0.4959432057616482 0.5335009880943957
O 0.2780933729731956 0.0013468071294724 0.5364572173215905
O 0.2219070547787609 0.4986541986568866 0.4635431754038137
O 0.7266192565987879 0.0040564290943834 0.4664997533623634
O 0.9999130160581586 0.7786757155928896 0.4594722241649265
O 0.4983197486877700 0.2859516298666804 0.4654887198865296
O 0.0016815346685135 0.2140487385021785 0.5345112368639562
O 0.5000857511022403 0.7213240526616360 0.5405267158500351

$La_{0.50}Sr_{0.50}FeO_3$ Pseudocubic Cell (-281.884 eV)
7.8613877501446314 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.8613877501446314 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.8613877501446314
Fe 0.7479674848667131 0.2513427323352957 0.9993442991664949
Fe 0.2475293968841257 0.7502814862904685 0.0005218747789968
Fe 0.2512556233210290 0.2472393467537941 0.9997247314788424
Fe 0.7513685527053653 0.7485870705063036 0.0008770555911184
Fe 0.7479605147681951 0.2511024548762748 0.4999386130882257
Fe 0.2493581792364736 0.7519265617084514 0.4996055887263324
Fe 0.2508131467707670 0.2471874667654816 0.5003042398051605
Fe 0.7520631285377988 0.7482566141563112 0.4995830983719429
La 0.5118465213696837 0.9816079939693267 0.7512204142037220
La 0.0104130367681279 0.4816737216734381 0.7516151144365821
La 0.4805377614837383 0.5086447663708995 0.2494960875956096
La 0.9838629157354006 0.0138402737176690 0.2480208535570085
Sr 0.9907550319707994 0.5091175374276702 0.2501403721348439
Sr 0.0106247875349013 0.9940897400626838 0.7494813509706688
Sr 0.5090965634248619 0.4897792103342198 0.7511820870245103
Sr 0.4940579754722592 0.0112883793486702 0.2486716965993168
O 0.7785822715149919 0.2653895401720163 0.2502948384743107
O 0.2856891143273401 0.7717813462775140 0.2390169444622714
O 0.2094927236994124 0.7170323148077884 0.7613268717728232
O 0.7155419409567898 0.2198402463790075 0.7487408279614272
O 0.2664351103428189 0.2776547271973371 0.7475917470221773
O 0.7677580053725279 0.7855575663066148 0.7385802028877606
O 0.7167867504994518 0.7088919885914535 0.2606059107723837
O 0.2214916148144894 0.2173328845254971 0.2525657047448462
O 0.2330533993040973 0.5062832175143299 0.0303252482237966
O 0.7285762335994903 0.9923799886463058 0.0266748135610086
O 0.7830381891444773 0.5077412539068504 0.9669940083930157
O 0.2786748038659397 0.9927373480734616 0.9653932586684491
O 0.9981238481153980 0.2330652270443565 0.9739152216805067
O 0.5112442361276095 0.7280623708071587 0.9688807320707653
O 0.9909683391898128 0.7812289866748898 0.0382205080560922
O 0.5014215654847334 0.2791406889803909 0.0307064620379123
O 0.7822351775199508 0.5080037927391814 0.5350569795911682
O 0.2814049625812771 0.9905033158559959 0.5357868215160053
O 0.2275215618644992 0.5129015385965232 0.4712541545405458
O 0.7332809216918932 0.9913877090869363 0.4664067862615582
O 0.0134984985959647 0.7863278748032698 0.4645191884694881
O 0.4987547734179643 0.2793030357153015 0.4681044006115513
O 0.0001701644970993 0.2344213327219293 0.5268896476888614
O 0.4867449026217940 0.7270662592789563 0.5324212150019321

$LaFeO_3$ 160-atom supercell (-1216.388 eV)
14.7744665146 0.0000000000 0.0000000000
2.0376793587 14.6332745352 0.0000000000
-6.3239562108 -9.7087762587 9.1669025408
Fe 0.0000000000000000 0.2500000000000000 0.2500000000000000
Fe 0.7500000000000000 0.0000000000000000 0.2500000000000000
Fe 0.5000000000000000 0.7500000000000000 0.2500000000000000
Fe 0.2500000000000000 0.5000000000000000 0.2500000000000000
Fe 0.7500000000000000 0.5000000000000000 0.7500000000000000
Fe 0.2500000000000000 0.0000000000000000 0.7500000000000000
Fe 0.5000000000000000 0.2500000000000000 0.7500000000000000
Fe 0.0000000000000000 0.7500000000000000 0.7500000000000000
Fe 0.8750000000000000 0.8750000000000000 0.0000000000000000
Fe 0.6250000000000000 0.6250000000000000 0.0000000000000000
Fe 0.3750000000000000 0.3750000000000000 0.0000000000000000
Fe 0.1250000000000000 0.1250000000000000 0.0000000000000000
Fe 0.6250000000000000 0.1250000000000000 0.5000000000000000
Fe 0.1250000000000000 0.6250000000000000 0.5000000000000000
Fe 0.3750000000000000 0.8750000000000000 0.5000000000000000
Fe 0.8750000000000000 0.3750000000000000 0.5000000000000000
Fe 0.2500000000000000 0.2500000000000000 0.5000000000000000
Fe 0.0000000000000000 0.0000000000000000 0.5000000000000000
Fe 0.7500000000000000 0.7500000000000000 0.5000000000000000
Fe 0.5000000000000000 0.5000000000000000 0.5000000000000000
Fe 0.0000000000000000 0.5000000000000000 0.0000000000000000
Fe 0.5000000000000000 0.0000000000000000 0.0000000000000000
Fe 0.7500000000000000 0.2500000000000000 0.0000000000000000
Fe 0.2500000000000000 0.7500000000000000 0.0000000000000000
Fe 0.1250000000000000 0.8750000000000000 0.2500000000000000
Fe 0.8750000000000000 0.6250000000000000 0.2500000000000000
Fe 0.6250000000000000 0.3750000000000000 0.2500000000000000
Fe 0.3750000000000000 0.1250000000000000 0.2500000000000000
Fe 0.8750000000000000 0.1250000000000000 0.7500000000000000
Fe 0.3750000000000000 0.6250000000000000 0.7500000000000000
Fe 0.6250000000000000 0.8750000000000000 0.7500000000000000
Fe 0.1250000000000000 0.3750000000000000 0.7500000000000000
La 0.8770962950000012 0.7705255750000006 0.1434292349999993
La 0.6270962950000012 0.5205255750000006 0.1434292349999993
La 0.3770962950000012 0.2705255750000006 0.1434292349999993
La 0.1270962950000012 0.0205255750000006 0.1434292349999993
La 0.6270962950000012 0.0205255750000006 0.6434292200000016
La 0.1270962950000012 0.5205255750000006 0.6434292200000016
La 0.3770962950000012 0.7705255750000006 0.6434292200000016
La 0.8770962950000012 0.2705255750000006 0.6434292200000016
La 0.3729036750000034 0.4794744249999994 0.8565707209999971
La 0.1229037049999988 0.2294744249999994 0.8565707209999971

La 0.8729037049999988 0.9794744249999994 0.8565707209999971
La 0.6229037049999988 0.7294744249999994 0.8565707209999971
La 0.1229037049999988 0.7294744249999994 0.3565707209999971
La 0.6229037049999988 0.2294744249999994 0.3565707209999971
La 0.8729037049999988 0.4794744249999994 0.3565707209999971
La 0.3729036750000034 0.9794744249999994 0.3565707209999971
La 0.2520962950000012 0.1086670760000032 0.6065707799999984
La 0.0020962950000012 0.8586670760000032 0.6065707799999984
La 0.7520962950000012 0.6086670760000032 0.6065707799999984
La 0.5020962950000012 0.3586670760000032 0.6065707799999984
La 0.0020962950000012 0.3586670760000032 0.1065707209999971
La 0.5020962950000012 0.8586670760000032 0.1065707209999971
La 0.7520962950000012 0.1086670760000032 0.1065707209999971
La 0.2520962950000012 0.6086670760000032 0.1065707209999971
La 0.9979037049999988 0.1413329390000015 0.3934292499999970
La 0.7479037049999988 0.8913329239999968 0.3934292499999970
La 0.4979037049999988 0.6413329239999968 0.3934292499999970
La 0.2479037049999988 0.3913329239999968 0.3934292499999970
La 0.7479037049999988 0.3913329239999968 0.8934292790000029
La 0.2479037049999988 0.8913329239999968 0.8934292790000029
La 0.4979037049999988 0.1413329390000015 0.8934292790000029
La 0.9979037049999988 0.6413329239999968 0.8934292790000029
O 0.1049529309999997 0.2203660759999977 0.3654131289999967
O 0.8549529309999997 0.9703660610000000 0.3654131289999967
O 0.6049529309999997 0.7203660610000000 0.3654131289999967
O 0.3549529309999997 0.4703660610000000 0.3654131289999967
O 0.8549529309999997 0.4703660610000000 0.8654131289999967
O 0.3549529309999997 0.9703660610000000 0.8654131289999967
O 0.6049529309999997 0.2203660759999977 0.8654131289999967
O 0.1049529309999997 0.7203660610000000 0.8654131289999967
O 0.1450470690000003 0.0296339390000000 0.6345868710000033
O 0.8950470690000003 0.7796339390000000 0.6345868710000033
O 0.6450470690000003 0.5296339390000000 0.6345868710000033
O 0.3950470690000003 0.2796339390000000 0.6345868710000033
O 0.8950470690000003 0.2796339390000000 0.1345868109999984
O 0.3950470690000003 0.7796339390000000 0.1345868109999984
O 0.6450470690000003 0.0296339390000000 0.1345868109999984
O 0.1450470690000003 0.5296339390000000 0.1345868109999984
O 0.2299529309999997 0.8645397419999981 0.3845868410000008
O 0.9799529309999997 0.6145397419999981 0.3845868410000008
O 0.7299529309999997 0.3645397419999981 0.3845868410000008
O 0.4799529309999997 0.1145397419999981 0.3845868410000008
O 0.9799529309999997 0.1145397419999981 0.8845868109999984
O 0.4799529309999997 0.6145397419999981 0.8845868109999984
O 0.7299529309999997 0.8645397419999981 0.8845868109999984
O 0.2299529309999997 0.3645397419999981 0.8845868109999984

O 0.0200470609999996 0.3854601979999970 0.6154131289999967
O 0.7700470690000003 0.1354601379999991 0.6154131289999967
O 0.5200470690000003 0.8854601979999970 0.6154131289999967
O 0.2700470690000003 0.6354601979999970 0.6154131289999967
O 0.7700470690000003 0.6354601979999970 0.1154131890000016
O 0.2700470690000003 0.1354601379999991 0.1154131890000016
O 0.5200470690000003 0.3854601979999970 0.1154131890000016
O 0.0200470609999996 0.8854601979999970 0.1154131890000016
O 0.8429599999999979 0.9647609590000030 0.1647810190000030
O 0.5929599999999979 0.7147610190000009 0.1647810190000030
O 0.3429599999999979 0.4647610190000009 0.1647810190000030
O 0.0929599999999979 0.2147610190000009 0.1647810190000030
O 0.5929599999999979 0.2147610190000009 0.6647810340000007
O 0.0929599999999979 0.7147610190000009 0.6647810340000007
O 0.3429599999999979 0.9647609590000030 0.6647810340000007
O 0.8429599999999979 0.4647610190000009 0.6647810340000007
O 0.4070400299999974 0.2852390409999970 0.8352190259999972
O 0.1570400000000021 0.0352389809999991 0.8352190259999972
O 0.9070400000000021 0.7852390409999970 0.8352190259999972
O 0.6570400000000021 0.5352390409999970 0.8352190259999972
O 0.1570400000000021 0.5352390409999970 0.3352190259999972
O 0.6570400000000021 0.0352389809999991 0.3352190259999972
O 0.9070400000000021 0.2852390409999970 0.3352190259999972
O 0.4070400299999974 0.7852390409999970 0.3352190259999972
O 0.4249799549999977 0.0531789770000017 0.5852190259999972
O 0.1749799250000024 0.8031789659999973 0.5852190259999972
O 0.9249799250000024 0.5531789659999973 0.5852190259999972
O 0.6749799250000024 0.3031789659999973 0.5852190259999972
O 0.1749799250000024 0.3031789659999973 0.0852190259999972
O 0.6749799250000024 0.8031789659999973 0.0852190259999972
O 0.9249799250000024 0.0531789770000017 0.0852190259999972
O 0.4249799549999977 0.5531789659999973 0.0852190259999972
O 0.8250200749999976 0.1968210189999979 0.4147810039999982
O 0.5750200749999976 0.9468210340000027 0.4147810039999982
O 0.3250200749999976 0.6968210340000027 0.4147810039999982
O 0.0750200749999976 0.4468210340000027 0.4147810039999982
O 0.5750200749999976 0.4468210340000027 0.9147809740000028
O 0.0750200749999976 0.9468210340000027 0.9147809740000028
O 0.3250200749999976 0.1968210189999979 0.9147809740000028
O 0.8250200749999976 0.6968210340000027 0.9147809740000028
O 0.2000200450000023 0.2852390409999970 0.6281989809999970
O 0.9500200749999976 0.0352389809999991 0.6281989809999970
O 0.7000200749999976 0.7852390409999970 0.6281989809999970
O 0.4500200450000023 0.5352390409999970 0.6281989809999970
O 0.9500200749999976 0.5352390409999970 0.1281989809999970
O 0.4500200450000023 0.0352389809999991 0.1281989809999970

O 0.7000200749999976 0.2852390409999970 0.1281989809999970
O 0.2000200450000023 0.7852390409999970 0.1281989809999970
O 0.0499799549999977 0.9647609590000030 0.3718009589999980
O 0.7999799250000024 0.7147610190000009 0.3718009589999980
O 0.5499799250000024 0.4647610190000009 0.3718009589999980
O 0.2999799549999977 0.2147610190000009 0.3718009589999980
O 0.7999799250000024 0.2147610190000009 0.8718009589999980
O 0.2999799549999977 0.7147610190000009 0.8718009589999980
O 0.5499799250000024 0.9647609590000030 0.8718009589999980
O 0.0499799549999977 0.4647610190000009 0.8718009589999980
O 0.0320400000000021 0.1968210189999979 0.6218009589999980
O 0.7820400000000021 0.9468210340000027 0.6218009589999980
O 0.5320400000000021 0.6968210340000027 0.6218009589999980
O 0.2820400000000021 0.4468210340000027 0.6218009589999980
O 0.7820400000000021 0.4468210340000027 0.1218008999999967
O 0.2820400000000021 0.9468210340000027 0.1218008999999967
O 0.5320400000000021 0.1968210189999979 0.1218008999999967
O 0.0320400000000021 0.6968210340000027 0.1218008999999967
O 0.2179599850000002 0.0531789770000017 0.3781990109999995
O 0.9679599999999979 0.8031789659999973 0.3781990109999995
O 0.7179599999999979 0.5531789659999973 0.3781990109999995
O 0.4679599999999979 0.3031789659999973 0.3781990109999995
O 0.9679599999999979 0.3031789659999973 0.8781989809999970
O 0.4679599999999979 0.8031789659999973 0.8781989809999970
O 0.7179599999999979 0.0531789770000017 0.8781989809999970
O 0.2179599850000002 0.5531789659999973 0.8781989809999970

$La_{0.75}Sr_{0.25}FeO_3$ 160-atom supercell, sqs arrangement (-1180.582 eV)

14.7714827069220096 0.0303336473686746 0.0298535258640774
2.0671112365864719 14.6082314146122254 -0.0307699878091586
-6.3240435709670866 -9.7243732375290204 9.1145691513134413

Fe 0.9995778086476714 0.2509749618837064 0.2512219694200561
Fe 0.7524848654584295 0.9996738515852643 0.2509603302630882
Fe 0.4996489792997066 0.7467736143355649 0.2472101779022650
Fe 0.2503009920572850 0.4999274304504868 0.2497151344042899
Fe 0.7522099007923146 0.5024723486183359 0.7541458491015177
Fe 0.2506808323134137 0.0003446151726810 0.7503823350103470
Fe 0.4997411349118834 0.2484738354943351 0.7496352445269135
Fe 0.9996840049389507 0.7496449472420900 0.7501331030391447
Fe 0.8740322176599445 0.8740929268569828 0.9997399702996381
Fe 0.6255258013903489 0.6252636066767878 0.0002797835955715
Fe 0.3770242298089778 0.3747707777838352 0.0013825899484155
Fe 0.1239370103050249 0.1243943368889238 0.0002057549655029
Fe 0.6291011882371413 0.1263235867103503 0.5027428974941269
Fe 0.1247666468145248 0.6248340282847452 0.4992198496642766
Fe 0.3764749618461946 0.8743870324459037 0.5014512227600327
Fe 0.8751043478071808 0.3750281135795911 0.4995732131552404
Fe 0.2491412060202639 0.2501063222615204 0.4999093636438604
Fe 0.9989389197651156 0.0003928880823390 0.4976145488482356
Fe 0.7495908697166442 0.7469932575414390 0.4977739913995263
Fe 0.5003794394697000 0.5040026134411070 0.5033153678913820
Fe 0.9981340033383150 0.5017567662219447 0.9982701419576021
Fe 0.5005346702364651 0.9990456730642359 0.0000341820771483
Fe 0.7489191867285592 0.2500451641455204 0.0005968240281127
Fe 0.2499997117331441 0.7471667620407696 0.9986089000128773
Fe 0.1233759512965940 0.8734810357669641 0.2487345294722841
Fe 0.8758841824783435 0.6252365020082641 0.2510928150198338
Fe 0.6252104482159954 0.3750347046302688 0.2475070327275312
Fe 0.3731044214941790 0.1252245060351852 0.2490921678397305
Fe 0.8754591759760921 0.1250644660300237 0.7494281062583710
Fe 0.3750373715071583 0.6266143212904306 0.7498347542001801
Fe 0.6232251248223536 0.8737925859331402 0.7480488725072315
Fe 0.1248217256238604 0.3741230604715441 0.7501707431365222
La 0.1247832227949000 0.0174343247667848 0.1411328317532955
La 0.3810259781776210 0.2709430584819502 0.1410352845409787
La 0.3806860373667902 0.7713724429311870 0.6415217860556331
La 0.1248459476803824 0.5164217225040121 0.6389386170895202
La 0.9955885205136669 0.6362189114071114 0.8872849916213293
La 0.7457973825699981 0.3874931046433829 0.8899405574100447
La 0.2498483672739739 0.8882177263812826 0.8891160200000514
La 0.2490203762993786 0.3911715805827946 0.3915753564279878
La 0.9960339731623726 0.1377543607527730 0.3902796553262494
La 0.7458386943309917 0.8843252933198292 0.3877575671612123

La 0.1230818912400735 0.7328022822539165 0.3600623867029718
La 0.6241082606703010 0.2371683279522920 0.3611110200909701
La 0.3729865474119641 0.9823048997867915 0.3607961873860978
La 0.3749546019805700 0.4820250783259750 0.8600256738155730
La 0.1260732834731939 0.2345735101529867 0.8623091070710609
La 0.8711594425526877 0.9845964184768526 0.8619524553953118
La 0.9982228918872572 0.3611539234356151 0.1081152410685783
La 0.7508278068108275 0.1122381678068286 0.1116173378244023
La 0.5034699538752249 0.8610171953960037 0.1103530635815571
La 0.2508628609455042 0.6105166217944394 0.1107489764351995
La 0.5038151516602764 0.3645248049918070 0.6137764621115829
La 0.2504878354525738 0.1095282288052685 0.6094690280829378
La 0.9999691104589742 0.8602482213914198 0.6088197236430882
La 0.7506347682528370 0.6105090129933991 0.6099542495130167
Sr 0.8737128963905295 0.7619688444188372 0.1362964540387328
Sr 0.6276030020325937 0.5120742733799123 0.1364856902364276
Sr 0.6257471850473032 0.0094774241837684 0.6343109646409140
Sr 0.8767915234824916 0.2628003328887679 0.6367453836962225
Sr 0.5019665734920904 0.1370946219141378 0.8865532393186157
Sr 0.5031279950427519 0.6363600558541703 0.3860060589768599
Sr 0.8722185288570423 0.4849943619174952 0.3604174139929837
Sr 0.6257321730618085 0.7381048993055963 0.8640157097335417
O 0.1059869986698812 0.2246105236446422 0.3716656646126168
O 0.8553876629557451 0.9802172536629238 0.3741214170457324
O 0.6154116051472737 0.7448260340794306 0.3781625064505243
O 0.3578733949603445 0.4739441339738827 0.3684207451691925
O 0.8558512862351381 0.4740814797353186 0.8690481518195917
O 0.3563057489301221 0.9742985335355940 0.8666852242489138
O 0.6161723239499152 0.2333289620230332 0.8692168157218086
O 0.1072366529452817 0.7252065849619704 0.8710421720725972
O 0.1412231414384316 0.0249382356165048 0.6329666066191694
O 0.8947400702538640 0.7787050754402706 0.6364355596192977
O 0.6395488072525338 0.5093655629069628 0.6190247182972056
O 0.3916099907636656 0.2747414295691715 0.6282696181792650
O 0.8921508680409355 0.2644906069472254 0.1211004489037860
O 0.3930444271895626 0.7771596067659140 0.1313485084115354
O 0.6442954112449443 0.0268679425943481 0.1374383665379243
O 0.1398185149902914 0.5200194404474006 0.1266070984925281
O 0.2310419331378423 0.8640993917160921 0.3817804053550271
O 0.9868305761220538 0.6186973169699603 0.3836158518522772
O 0.7326118149205392 0.3664539648838516 0.3834048539892266
O 0.4691288269293170 0.1137812460715269 0.3729916480133267
O 0.9836278228202477 0.1140074002717132 0.8875866958046245
O 0.4803057409530301 0.6126970282463626 0.8788217378117520
O 0.7375839879510937 0.8751090945460653 0.8868350091913986
O 0.2321796974908441 0.3656033108572675 0.8836407610918720

O 0.0197203116799760 0.3850632913751582 0.6173126105673402
O 0.7658862778855514 0.1293310352894022 0.6130869943308120
O 0.5120229085946795 0.8830422910326842 0.6212849245927022
O 0.2700567709693174 0.6384419853736037 0.6173043249279507
O 0.7629798610019926 0.6277913806905415 0.1167668509194123
O 0.2759381684045497 0.1374172798669011 0.1222353966228199
O 0.5122856216625061 0.3836359203193769 0.1213262873423791
O 0.0189948613016183 0.8834312350039297 0.1150129457712581
O 0.8391298368765334 0.9639185703807402 0.1600543311082927
O 0.5848759873865887 0.7139593370285422 0.1571202055163526
O 0.3334825176792046 0.4581896948807392 0.1553299880203742
O 0.0935208575471519 0.2110233868120290 0.1645318686653788
O 0.5866139866926858 0.2127532679994911 0.6492647331794690
O 0.0914440527130780 0.7112148227506896 0.6625252095458063
O 0.3337853068010557 0.9586241917684515 0.6553385016339841
O 0.8368197136825313 0.4608756450018186 0.6578232799903205
O 0.4093816530181484 0.2911984546502737 0.8388361706793234
O 0.1602972450644203 0.0356998931037727 0.8401367488189718
O 0.9100130402508450 0.7898376270296196 0.8387168511359698
O 0.6630180672529402 0.5366644245811755 0.8409404658620617
O 0.1592580789568946 0.5354307872653886 0.3362866895712527
O 0.6553052076992846 0.0454521278089581 0.3443435103805625
O 0.9112677486379751 0.2848914722942327 0.3383859658929551
O 0.4102620450980354 0.7935704452133364 0.3399138356459116
O 0.4232685828619471 0.0565624967654085 0.5902632711625369
O 0.1759372346019738 0.8048656863479403 0.5897765438717051
O 0.9280454795811625 0.5563338935419266 0.5970554680386989
O 0.6691455944453860 0.2963261982082581 0.5827246415836768
O 0.1768135974679753 0.3021360688652434 0.0901546498890634
O 0.6749216493943723 0.8103369101647452 0.1008712623056959
O 0.9314439236508512 0.0545279317239429 0.0924673291575195
O 0.4233974721622589 0.5561913031919163 0.0907977701990156
O 0.8225514166498040 0.1933146300684732 0.4035490564392242
O 0.5709743462632298 0.9556456908350976 0.4060164289190752
O 0.3155097493324547 0.6955032354267118 0.4070967828433310
O 0.0771671304101633 0.4446319063541803 0.4110224441944071
O 0.5685879291910275 0.4413273209816048 0.8973838337347150
O 0.0784485244862447 0.9460671079401389 0.9146082760495612
O 0.3163583780474527 0.1956826075899208 0.9081944752880404
O 0.8242604441796032 0.6925484067521560 0.9013488243938175
O 0.2032431613229272 0.2893051825827796 0.6310565331807890
O 0.9510305775299689 0.0428063555573539 0.6369937294956947
O 0.7037738116474302 0.7974011697845582 0.6356995405764315
O 0.4447152506012783 0.5320312079455913 0.6198913692746316
O 0.9509625183113208 0.5404616588071862 0.1291631690706465
O 0.4502000700600953 0.0357826135042386 0.1261891725739062

O 0.6979018312987004 0.2883073752422067 0.1269898985451937
O 0.2030279500375065 0.7905641651327314 0.1310994970249146
O 0.0542474598283561 0.9649644222683574 0.3757194764640935
O 0.8074015670283601 0.7141815997749764 0.3788773153093684
O 0.5485266781428896 0.4514228498279050 0.3708446298778667
O 0.2941195403638077 0.2124120512907166 0.3690686586360281
O 0.8103177011571779 0.2132321775308512 0.8716015096004913
O 0.2975353146271872 0.7105766966390381 0.8691933567820429
O 0.5520672677907400 0.9578279983492427 0.8749089349177598
O 0.0540857456463679 0.4646437982125771 0.8758670161834919
O 0.0409430463311765 0.1939677606437525 0.6217535813416780
O 0.7961656605995683 0.9534607757365552 0.6291752382824721
O 0.5395352331034867 0.6944438504749032 0.6253191743259512
O 0.2828583795921649 0.4471287304419455 0.6211564985204883
O 0.7930652899807337 0.4363399493106327 0.1151748536206918
O 0.2848875504873067 0.9522100317754871 0.1222678451405053
O 0.5381034979791399 0.1941002008519683 0.1285176182535155
O 0.0390002737359579 0.6940723581687177 0.1197626619140601
O 0.2153680775977908 0.0537653835818866 0.3777512750688222
O 0.9644478756479826 0.8080274503855680 0.3828883529435461
O 0.7085738235545389 0.5592809641280932 0.3853816656412059
O 0.4604844180047706 0.2950382565060931 0.3735649417510596
O 0.9652673436668319 0.2973156035228693 0.8775706610837294
O 0.4607783796823779 0.8067057441799890 0.8807110578781413
O 0.7144820515693532 0.0610029657493304 0.8830714441288701
O 0.2166497272354475 0.5536137481741451 0.8787718311748919

$La_{0.50}Sr_{0.50}FeO_3$ 160-atom supercell, sqs arrangement (-1128.921 eV)
14.6917432003535264 0.1016977892745896 0.0374737724710164
2.1270233011774762 14.5952306276325725 -0.0543041150731161
-6.3320582128541609 -9.7546688768502836 9.1006926372808898
Fe 0.0028013560091580 0.2514133393612212 0.2528217762540379
Fe 0.7482802016525909 0.9994093307998995 0.2498605994763707
Fe 0.5003395545322888 0.7505046371452195 0.2511596809715044
Fe 0.2526317364988699 0.5028070618339768 0.2545362201952699
Fe 0.7481416087865824 0.4990688833329742 0.7498832681900538
Fe 0.2518656876357284 0.9990720167724021 0.7482343469239794
Fe 0.4994032540727531 0.2454492610738654 0.7457165668365562
Fe 0.9987288579887235 0.7450500800148987 0.7429329659757684
Fe 0.8757842616638811 0.8728152336139701 0.0002877621831274
Fe 0.6289857775523018 0.6264100858865760 0.0023491604525603
Fe 0.3744039000233030 0.3746461005303985 0.0009598127005788
Fe 0.1233622385418869 0.1283889280182393 0.0003552759354974
Fe 0.6257469623777610 0.1286049264597509 0.5038664242766089
Fe 0.1253015796276316 0.6236724292272129 0.4975388274783299
Fe 0.3734541211853397 0.8739307310497537 0.5011650772125549
Fe 0.8762524510754730 0.3743913267941750 0.4987139798352871
Fe 0.2480736384043922 0.2465906386712149 0.4955494427274090
Fe 0.0038195867033792 0.9997566160529061 0.4974713886746613
Fe 0.7472155290877112 0.7463073739431252 0.5003806235013357
Fe 0.4993121076184508 0.5028248844228784 0.5016286837485637
Fe 0.0017806076796489 0.4999955525036555 0.9954299055377120
Fe 0.4983011351853293 0.0006362208167943 0.9981634187037116
Fe 0.7481879681508090 0.2476053950073833 0.9988974857841200
Fe 0.2525667023733718 0.7488826847288905 0.0002892954874412
Fe 0.1259484706503571 0.8752572006973978 0.2494537525918261
Fe 0.8711328128647224 0.6231351264545708 0.2502326946847333
Fe 0.6234857161521248 0.3727622750784221 0.2469930093019101
Fe 0.3787892334282361 0.1252791268508986 0.2560400273637171
Fe 0.8724848138508534 0.1250536921020782 0.7517968239119028
Fe 0.3736805655610169 0.6275409294132217 0.7479488650225790
Fe 0.6209625049849947 0.8710498748818694 0.7448943977383991
Fe 0.1280273312447378 0.3759922353830518 0.7484358090928325
La 0.6214407810207732 0.5106023334067729 0.1333248752606977
La 0.3792658480821629 0.2609679125554507 0.1358827598527910
La 0.6217825956623457 0.0080633848440144 0.6326280062659961
La 0.8747846929635088 0.2578483147851784 0.6293745618521314
La 0.2507274263957697 0.8826544815707251 0.8872890378879745
La 0.7491916093598476 0.8829892657103642 0.3838658576080149
La 0.1261791204020426 0.7418539016292556 0.3634140021978922
La 0.8715327857975481 0.4801658169103717 0.3582165625677334
La 0.3722936224457811 0.9885128895336095 0.3633594428399718
La 0.3744341031329128 0.4879637873876419 0.8619404100580041

La 0.1267413439813865 0.2477039020375926 0.8671700833084799
La 0.8712983054042809 0.9866123217996403 0.8663134762321079
La 0.0020411133663316 0.3685923194153204 0.1183929002845119
La 0.7454607648665643 0.1082136785145735 0.1114617548469070
La 0.0024293770497366 0.8682854182827668 0.6169590940331489
La 0.7477872700498267 0.6111309531195559 0.6160912132928971
Sr 0.1255104843339367 0.0066545026012435 0.1317450591629594
Sr 0.8741870738338733 0.7575897262522915 0.1277229858255495
Sr 0.3769381774961147 0.7570038289517100 0.6338321868831400
Sr 0.1290783613929847 0.5069631082521369 0.6309459714451080
Sr 0.0032052897920423 0.6317233449188251 0.8822147647230381
Sr 0.7500696612046980 0.3862438655349223 0.8853085419355082
Sr 0.4966620937467425 0.1292272604491629 0.8803180506963173
Sr 0.4948272154213100 0.6289628900052975 0.3812109117355220
Sr 0.2539468246435845 0.3811021170060656 0.3873762844609274
Sr 0.0009987619946656 0.1291963038000148 0.3790354195325563
Sr 0.6228293941582947 0.2428612485377712 0.3695905531030093
Sr 0.6231139256776004 0.7424426528097428 0.8691446535264973
Sr 0.5026015294719528 0.8714711598590057 0.1183003674869951
Sr 0.2513828729464151 0.6204579327032036 0.1182429256810877
Sr 0.5026361295864987 0.3740277509181738 0.6213881900622553
Sr 0.2521913318156095 0.1180696885315271 0.6160074387378103
O 0.1162726914014911 0.2405885347433028 0.3734326077337400
O 0.8680622471259767 0.9846048536449317 0.3878955937652790
O 0.6129981009258714 0.7244357131065939 0.3705267516535002
O 0.3603882744077467 0.4751213999778088 0.3624696049716363
O 0.8697141458675333 0.4794722257763269 0.8712584328170507
O 0.3542140302835719 0.9822710497696931 0.8726142862343664
O 0.6062720484161943 0.2294139916210725 0.8639991862056888
O 0.1099787949201740 0.7425989735246006 0.8674631590658279
O 0.1327389689001279 0.0296001727067718 0.6375368129549983
O 0.8967810392918381 0.7740046792726929 0.6340415376820161
O 0.6374203420831464 0.5092163721622498 0.6230334000248590
O 0.3973701680098500 0.2697441987575573 0.6365245321014967
O 0.8895274611583659 0.2617966899663102 0.1213572697924903
O 0.3894742265731850 0.7746559352286937 0.1329021807476849
O 0.6341679483406182 0.0158964768364100 0.1279864727096367
O 0.1298412773589419 0.5189753841639373 0.1261327860228647
O 0.2369162631555071 0.8552768234109251 0.3670974164803127
O 0.9748850029256531 0.6138845399949560 0.3758450837122211
O 0.7418057211792473 0.3649163447994894 0.3854797581461256
O 0.4889241400489794 0.1058738490143156 0.3757360487975134
O 0.9781268440061837 0.1172862165629596 0.8853306084973980
O 0.4963809661925751 0.6167371165537929 0.8928973225170580
O 0.7452727576214144 0.8695927180463485 0.8880663127946846
O 0.2387796978948202 0.3599696189751214 0.8713769520414871

O 0.0062368825095902 0.3772883560805624 0.6075938424855352
O 0.7710409991354723 0.1328581926831092 0.6231028046578828
O 0.5153371111059499 0.8859736628100734 0.6200460837241906
O 0.2567281818886542 0.6386869534442141 0.6237443187340190
O 0.7650842863946323 0.6475312275514824 0.1369282817819055
O 0.2564770645957282 0.1385781266874062 0.1072373561533624
O 0.5161644141952877 0.3905970587990524 0.1245989315456839
O 0.0056658509699119 0.8850561941525186 0.1172840311522094
O 0.8262089093312710 0.9557195281198432 0.1546122927266964
O 0.5862898553764566 0.7086354050799599 0.1667309913087180
O 0.3243016919150321 0.4446707957699090 0.1399899746632940
O 0.0842955927673188 0.2103904488796289 0.1464070805440159
O 0.5832941493401833 0.1986602489274176 0.6534637746814624
O 0.0801627068373207 0.7181331628176792 0.6583706861576815
O 0.3251914989876568 0.9507612284892701 0.6429488088069064
O 0.8356139278906554 0.4468935794608981 0.6425505155982023
O 0.4252784585463161 0.3048978813200023 0.8514461572006624
O 0.1551463692259105 0.0529445517044991 0.8487943708921790
O 0.9164557320939224 0.7958709032128013 0.8362526040966429
O 0.6785258899151998 0.5546422023838460 0.8623128588822269
O 0.1602393534301569 0.5477561417893355 0.3435208079803260
O 0.6790720284914329 0.0421375069733969 0.3562089534044404
O 0.9070394319922812 0.2895241727503546 0.3395279717435287
O 0.4236610667796015 0.8001738827377807 0.3471348609862446
O 0.4282658671497259 0.0505706497704210 0.5893082986095806
O 0.1661691792824342 0.8088647761874839 0.5929692715812394
O 0.9249778624972436 0.5553216893241526 0.5910862382568709
O 0.6868831781900937 0.3062681431975562 0.6076900569805943
O 0.1655995786140991 0.3006707971742060 0.0844710909886004
O 0.6830962743315681 0.8114755039820878 0.1121752572613275
O 0.9240465444908921 0.0513626731969907 0.0943666512435897
O 0.4315960840365278 0.5603815733185087 0.0967415990708460
O 0.8176883521004967 0.1813596743695385 0.3962148914159371
O 0.5790777255250461 0.9401736803640546 0.4073985571755472
O 0.3167438645678828 0.6918076312711108 0.3954236190703995
O 0.0593988800773246 0.4451202056333941 0.3935005637333120
O 0.5778022651820862 0.4575218330409854 0.9161799370894741
O 0.0754934973668142 0.9597172730239478 0.9087256409484965
O 0.3203560416109639 0.1939032033757258 0.9035140374449355
O 0.8247689630341242 0.6938899436137334 0.8891306521449849
O 0.2006557167626895 0.3025304571042966 0.6306861126800527
O 0.9477082255348037 0.0544464055874130 0.6488961767355903
O 0.7056703793519432 0.7929475852221870 0.6362476937729156
O 0.4432132263617490 0.5538593220261632 0.6349269484406577
O 0.9438555268429525 0.5530817804847956 0.1434509584065893
O 0.4347636602070324 0.0520926368344448 0.1278339507281387

O 0.7008593829339631 0.2890385662195314 0.1297775847521763
O 0.1967902587896262 0.8042117375216051 0.1272441198820502
O 0.0572048840840580 0.9466963511114983 0.3703431734017713
O 0.8044561571185724 0.7073987450171657 0.3708927602178065
O 0.5551554874093156 0.4479672635008143 0.3708691208448940
O 0.3087876484286127 0.1955746991279312 0.3677058732646614
O 0.8024576723651649 0.2008385538710229 0.8641367017405770
O 0.3070311109809367 0.7037505212852722 0.8700475120843834
O 0.5585852797203472 0.9541716545085706 0.8771866230995400
O 0.0523917356185422 0.4391781613384538 0.8596920710311267
O 0.0375959091677984 0.1871217874445676 0.6185461972192314
O 0.7884299920903359 0.9399648030420877 0.6202180148067882
O 0.5482440788607121 0.6905000873525395 0.6225222315531411
O 0.3072573064590287 0.4516741048752451 0.6375250963294619
O 0.7858181263152630 0.4418434058058267 0.1245538931432151
O 0.2936632226050833 0.9492085881084620 0.1177404129121769
O 0.5395828459717578 0.1928572171490828 0.1203273448317859
O 0.0419969403315648 0.6847094545149233 0.1176957844852637
O 0.2097985092411889 0.0563891512283945 0.3782957190020824
O 0.9667534669155913 0.8201271259172174 0.3990177937673707
O 0.7157812313687657 0.5539915124750365 0.3822630078173432
O 0.4474043407857806 0.2992290365645687 0.3704145245034027
O 0.9633341913914393 0.3169021096186526 0.8925942832879556
O 0.4500815436636998 0.8032018289298009 0.8768564629283091
O 0.7088822843256537 0.0535133741394915 0.8735550336592368
O 0.2071788014721321 0.5577950624301948 0.8751713701181103