Supplemental Information

Table of Contents

Computational Search Method – *Genetic Algorithm*

Genetic algorithm studies traditionally represent a crystal by a list of N atomic Cartesian coordinates, requiring no prior information about the system aside from the composition and volume of the unit cell. The crystal structures for this study were similarly represented by the Cartesian coordinates of each lattice site[1] in the fcc undoped CeO_2 lattice. A vacancy is created for every two dopant atoms so, specifically, the genetic representation of a generic lanthanide-doped ceria (LDC) structure is constructed by assigning N dopant atoms to distinct ceria lattice sites and N/2 vacancies to distinct oxygen sites. A collection of LDC structures, or "genes", is herein referred to as a "population". The initial populations are constructed by substituting dopants and oxygen vacancies at randomly selected Ce and O sites on the undoped lattice. For example, the 3.3% and 6.6% Ln_2O_3 concentrations are built by introducing one and two oxygen vacancies, respectively, to a 96-atom CeO_2 2x2x2 supercell.

For structure evolution, the number of atoms was kept constant for the duration of the procedure wherein, at each step, randomly chosen mutation or mating operations were used to combine structural motifs of one or two randomly chosen "parent" genes. The mating/mutation operations were designed to accommodate both dopant- and vacancy-type defects and preserve the lanthanide coordinates from the original $F_{m\text{-}3m}$ symmetry lattice. The mating and mutation operations used in this study were the following: i) randomly perturbing the Cartesian coordinates of a chosen subset of atoms from the parent to make the offspring; ii) swapping individual Cartesian coordinates of a randomly chosen subset of Ln atoms with those of a randomly chosen subset of Ce atoms; iii) swapping individual Cartesian coordinates of a randomly chosen subset of

oxygen atoms with those of a randomly chosen subset of oxygen vacancies; and iv) swapping the Ce/Ln lattice sites of one parent structure with those of the other parent structure. Only one randomly chosen mating/mutation operation was used to generate a single offspring. Occasionally these mating procedures generated physically unreasonable crystal structures, thus offspring structures were only added to the next generation if all atomic pairs were at least 1.0Å apart, otherwise the same mating operation was repeated. The resulting offspring structures are given a twenty-five percent chance to mutate further through geometry perturbations. Specifically, this perturbation involves randomly selecting a non-empty pool of physically relevant lattice sites, by cycling through each atom and giving it a $1/N_T$ chance of being selected (N_T is the total number of atoms), and randomly perturbing each of their x, y, and z Cartesian coordinates by a maximum of 0.2Å.

The 'fitness' of a candidate structure, the metric that determines how well the structure fits the desired profile, was determined from its relative lattice energy to the lowest-energy structure in its population, as derived from classical polarizable force fields. The population of subsequent generations was created in the following manner: First, the fittest structures were promoted, unperturbed, to the next generation, usually those in the top 15 percentile. To generate the rest of the population, fit structures were preferentially chosen as parent structures by selecting them from a Boltzmann weighted probability distribution.[2] The exponential term stems from the relative lattice energies, scaled by an appropriate temperature to allow at least a 25% chance to select half of the promoted structures. Unphysical structures are screened out during the mating process

and the offspring structures are optimized, under variable cell conditions at zero pressure, before evaluating their fitness.[3]

Force Field Parameters

We used the GULP simulation package[4] for all classical molecular mechanics calculations, using the Buckingham potential to model short range dispersion pair-wise interactions, Ewald's method[5] to sum the long-range Coulombic interactions, and the shell model[6] to account for the polarizability of the O^{2-} ions. The oxygen shell had a charge of -2.08 e and was tied to the atomic core by a 27.29 eV/Å^2 spring constant. The Buckingham parameters, shown in Table A, were taken from Balducci et al.[7] and Senyshyn et al.[8]. Equation [1] shows the functional form of the Buckingham potential. The functions were evaluated between 0.5 and 10 Å for Ce-O and O-O pairs, and between 0.5 and 6 Å for Sm-O pairs. The elevation of the lower cutoff from 0.0 Å to 0.5 Å was employed to help efficiently eliminate unphysical structures from our genetic algorithm; it should in no way affect the energies of the low-energy structures. The force field was benchmarked and validated with first principles DFT calculations on 3.2% SDC by verifying that the order (by fitness) of selected structures was similar with both methods.

Table A. Buckingham parameters for interatomic potential calculation

Species	***A (eV)***	***ρ (Å)***	***C (eV Å^6)***
O^{2-} - O^{2-} [ref. 7]	22764.3	0.149	27.89
Ce^{4+} - O^{2-} [ref. 7]	1986.8	0.3511	20.40
Sm^{3+} - O^{2-} [ref. 8]	4040.9	0.3034	0.0

$$S_{ij} = Ae^{\left(-r_{ij}/\rho\right)} - \frac{C}{r_{ij}^6} \qquad [1]$$

Estimate of Vacancy-Vacancy Association Energy

A rough estimate of vacancy-vacancy association energies with the force field used in this study in 1.9% SDC structures is shown in Figure A1. The estimates were calculated by setting up three thousand sets of calculations in which four Sm atoms and two vacancies are distributed about the simulation cell. In each set, the four Sm atoms are placed at the same randomly chosen Ce lattice sites and kept constant while the two vacancies are placed at predefined oxygen sites such that they sample the vacancy-vacancy distance range shown in Figure A1. The energies are zeroed to the lowest energy configuration within each set and although the long-range electrostatic Sm-vacancy interactions are likely not consistent within each set, their effects are assumed to balance out over the series' entirety. Overall, the results do suggest a general repelling of the oxygen vacancies as they are brought closer together, becoming particularly repulsive below 6 Å, and sport a locally favored vacancy-vacancy distance between 6 and 8 Å. The apparent stabilization of vacancy-vacancy interactions beyond 8.5 Å in Figure A1 is an artifact of the random configurational sampling used to generate the plot, the lowest energy structure recovered from the procedure was duly noted to have a ~6.1 Å vacancy-vacancy distance. It can further be rationalized that vacancy-vacancy distances between 6 and 8 Å are stabilized over their periphery by Sm-vacancy interactions. We note that such vacancy-vacancy distances are in fact observed in all the low-energy configurations recovered at low concentrations and are characteristic of the aforementioned anisotropic defect distributions.

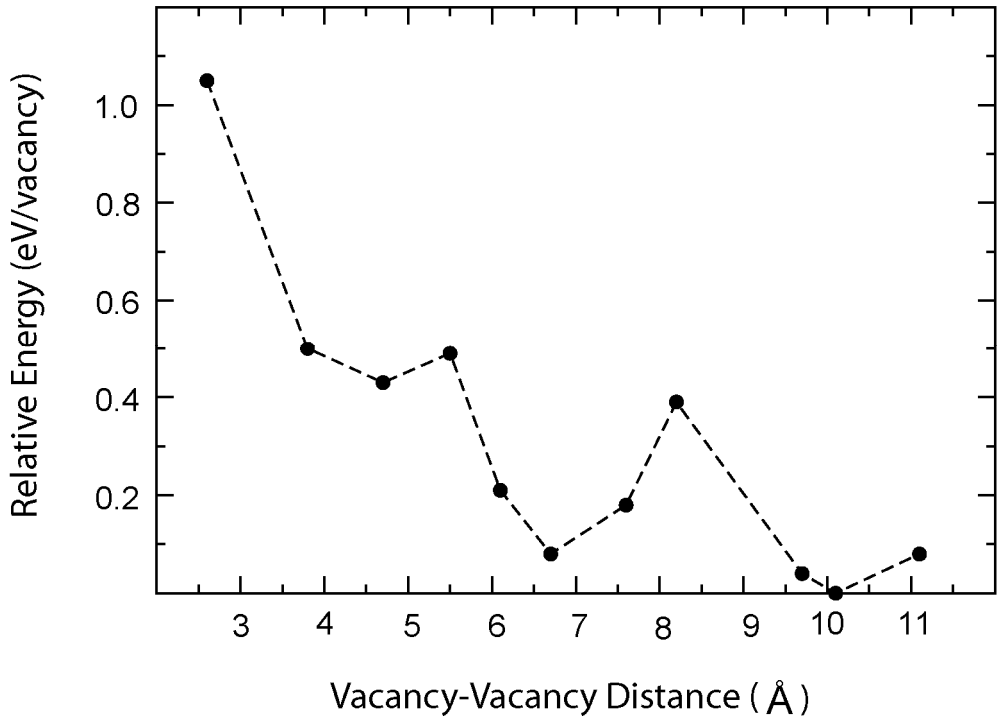

Figure A1. Estimate of vacancy-vacancy association energies; relative energies as a function of vacancy-vacancy distance in 1.9% SDC simulation cells, averaged over 3000 randomly generated configurations.

3.8% SDC

```
Sm Ce O
1.000000
       16.321487      -3.7e-05       -0.001005
       -3.5e-05       16.317447      0.004658
       -0.001004      0.004672       16.312984
8 100 212
Direct
       0.344398       0.670935       0.985437
       0.008116       0.502817       0.151506
       0.171659       0.668233       0.487334
       0.168874       0.510472       0.658643
       0.341693       0.336382       0.31969
       0.173168       0.002968       0.819496
       0.340228       0.505245       0.818762
       0.008439       0.335871       0.653629
       0.00746        0.004327       0.985099
       0.007068       0.002708       0.319053
       0.005999       0.003918       0.652346
       0.002246       0.331146       0.991174
       0.173507       0.33527        0.150973
       0.508012       0.502705       0.653601
       0.008549       0.669601       0.320372
       0.006209       0.671237       0.650334
       0.341          0.002126       0.31939
       0.673589       0.836561       0.8195
       0.50793        0.502656       0.984133
       0.004454       0.334481       0.317201
       0.347633       0.331333       0.657248
       0.003467       0.669289       0.987482
       0.346704       0.67704        0.323803
       0.345387       0.663117       0.646474
       0.6745         0.003146       0.986122
       0.674444       0.003417       0.319109
       0.674385       0.002933       0.652422
       0.675373       0.336078       0.985866
       0.675069       0.33631        0.319295
       0.673258       0.335843       0.65269
       0.675004       0.669247       0.985925
       0.674668       0.669874       0.318553
       0.673555       0.669481       0.652601
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       0.341283       0.171051       0.484073
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       0.346363       0.507003       0.476695
       0.50657        0.33506        0.484154
       0.341162       0.334205       0.984058
       0.341336       0.170284       0.153176
       0.345614       0.842004       0.82444
       0.67429        0.169489       0.152696
       0.67425        0.170185       0.485603
       0.674956       0.169945       0.819079
       0.673849       0.502831       0.151814
       0.674          0.502576       0.484902
       0.675648       0.503214       0.818985
       0.674719       0.836202       0.152289
       0.674679       0.837034       0.486031
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       0.173009       0.005294       0.483645
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0.341982	0.836301	0.15069
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0.507581	0.003435	0.152638
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8.0% SDC

```
Sm Ce O
1.000000
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        0.002496      -0.003064      16.338278
16 92 208
Direct
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        0.023753       0.525044       0.834436
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        0.848062       0.689072       0.828572
        0.020161       0.855898       0.156379
        0.01653        0.022345       0.66194
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        0.928945        0.575918        0.736901
        0.763502        0.391432        0.405256
        0.76965         0.232453        0.724603
        0.767276        0.575303        0.07153
        0.767383        0.568667        0.402323
        0.767595        0.578364        0.741424
        0.772962        0.908924        0.061859
        0.769355        0.909958        0.406936
        0.759998        0.93729         0.739278
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17.4% SDC

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Sm Ce O
1.000000
       16.397693      0.005651       -0.026748
       0.005581       16.397594      0.005657
       -0.026777      0.005641       16.392595
32 76 200
Direct
       0.612142       0.498567       0.498799
       0.770746       0.007135       0.841512
       0.110704       0.671631       0.499648
       0.779174       0.834193       0.334223
       0.779088       0.66823        0.837938
       0.275529       0.999328       0.995691
       0.609004       0.335105       0.999858
       0.10881        0.166888       0.993184
       0.613278       0.668069       0.330515
       0.610773       0.167881       0.164455
       0.94498        0.338438       0.329617
       0.942511       0.163358       0.831322
       0.281629       0.168841       0.498581
       0.280832       0.326603       0.664876
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0.777281	0.333527	0.167004
0.446372	0.668043	0.161793
0.937949	0.503734	0.173118
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0.114647	0.329799	0.832869
0.273106	0.668303	0.665576
0.437463	0.994213	0.828479
0.443929	0.164558	0.329916
0.44002	0.162808	0.668447
0.612576	0.8394	0.834427
0.108853	0.834986	0.658867
0.111577	0.50029	0.325353
0.942916	0.665105	0.00159
0.781191	0.001228	0.499324
0.951022	0.005191	0.658635
0.778071	0.501665	0.667103
0.618235	0.995593	0.007391
0.44483	0.50168	0.9976
0.946054	0.996393	0.991564
0.93808	0.32128	0.991999
0.284494	0.169009	0.839783
0.940126	0.340074	0.672631
0.95123	0.676599	0.332117
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0.619352	0.501149	0.842387
0.279415	0.0025	0.330779
0.281505	0.99544	0.657885
0.271952	0.334278	0.001421
0.277751	0.325798	0.325567
0.277844	0.661203	0.004103
0.273801	0.663585	0.326516
0.118994	0.490577	0.665156
0.446547	0.659583	0.821813
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0.611788	0.175598	0.824453
0.950119	0.173973	0.167699
0.620207	0.330193	0.65818
0.60516	0.672123	0.992232
0.439401	0.172008	0.005571
0.615999	0.655902	0.671808
0.937123	0.163106	0.488718
0.109498	0.663792	0.163104
0.952411	0.497808	0.507131
0.94599	0.83558	.165747
0.935729	0.830206	0.505406
0.273646	0.164719	0.162446
0.451932	0.326203	0.505867
0.440502	0.329175	0.836677
0.276759	0.500617	0.167674
0.269892	0.506231	0.49964
0.27843	0.499241	0.831731
0.274699	0.830374	0.49769
0.270895	0.839902	0.826378
0.610051	0.157971	0.506727
0.439781	0.007097	0.159932
0.616388	0.82338	0.164107
0.613233	0.840424	0.488548
0.112175	0.162319	0.333327
0.117074	0.009088	0.501987
0.104603	0.993127	0.835134
0.114862	0.328648	0.170851
0.120605	0.336629	0.489713
0.12071	0.670878	0.835412
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0.44945	0.843505	0.00242
0.439261	0.658986	0.493523
0.604401	0.497049	0.165375
0.281255	0.83307	0.160658
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0.774136	0.33228	0.830132
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0.119711	0.831439	0.323713
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```

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