

Supplementary Information

Reduced Ceria Nanofilms from Structure Prediction

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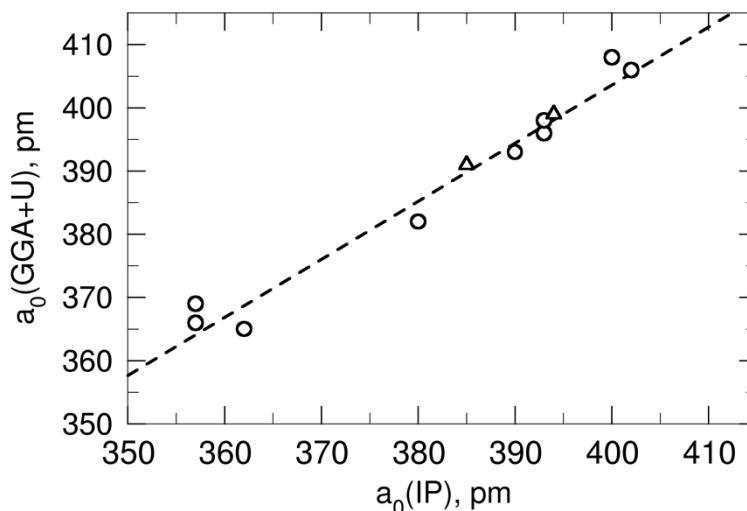


Figure S1. The correlation between GGA+U and IP calculated lattice parameters per Ce_2O_3 unit in films (circles) and bulk (triangles). The linear regression $a_0(\text{GGA+U}) = 0.92 a_0(\text{IP}) + 36.33$ yields $R^2 = 0.971$.

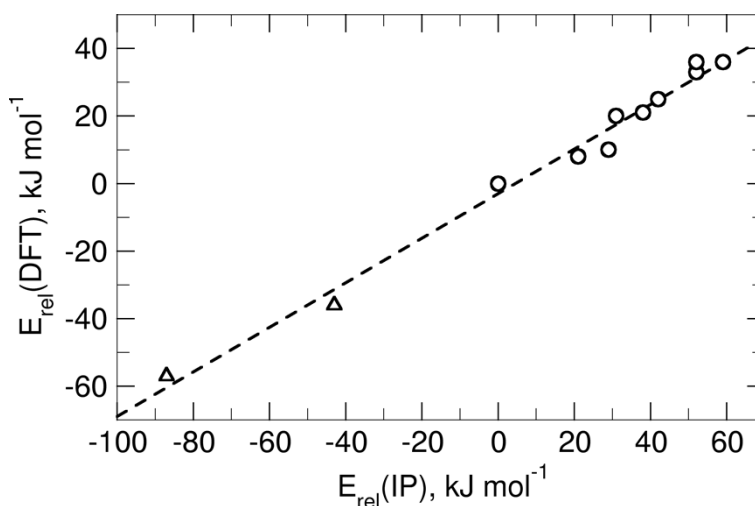


Figure S2. The correlation between GGA+U and IP calculated relative energies per Ce_2O_3 unit (with respect to those of bixbyite films) in films (circles) and bulk (triangles). The linear regression $E_{\text{rel}}(\text{GGA+U}) = 0.66 E_{\text{rel}}(\text{IP}) - 2.90$ yields $R^2 = 0.988$.

Structures of NF1-NF4 films (data in Å)

NF1

Periodic vectors

7.1301908000000003 0.0000000000000000
3.5363129000000000 6.1250736000000003

XYZ coordinates

Ce	9.46712857	4.13966014	3.93855472
Ce	2.35346419	0.46489039	3.942839
Ce	5.45986467	2.30361205	3.87764717
Ce	6.72125257	0.02376832	10.11803107
Ce	3.61173523	2.29614496	10.34851579
Ce	4.68483395	4.57405493	6.94204893
Ce	4.70737074	0.02541884	6.94188828
Ce	7.79435128	2.30167829	6.71156421
Ce	6.69871577	4.57240441	10.11819172
Ce	1.93896148	0.45816924	13.12152528
Ce	9.05262586	4.13293898	13.117241
Ce	5.94622185	2.29421119	13.18243283
O	4.70301931	0.02799385	4.17588623
O	4.68341169	4.57137227	4.18445916
O	3.34657593	2.30379652	2.92597704
O	6.99603524	0.37996922	7.78626953
O	9.48377329	4.10053007	6.20000542
O	4.41004768	4.21786015	9.27385047
O	5.41505976	2.29981103	6.12569875
O	7.85757797	2.29919755	4.27947807
O	2.3726452	0.50384791	6.2046905
O	4.42974876	0.3807003	9.27458087
O	1.92231323	0.49729318	10.86011458
O	6.97634128	4.21712907	7.78553913
O	6.72267836	0.0264571	12.87566084
O	8.05951058	2.29402672	14.13414296
O	6.70307073	4.56983552	12.88423377
O	9.03344132	4.09397534	10.8554295
O	3.54850854	2.2986257	12.78064193
O	5.99102675	2.29801222	10.93442125

NF2

Periodic vectors

13.6368628504789005 0.0000000000000000
-6.8083514918638501 11.7924106996955995

XYZ coordinates

Ce	6.75649	0.0343	1.78428
Ce	-0.24999	4.03896	1.76406
Ce	3.13821	1.87101	1.77826
Ce	-1.26082	5.79787	4.90386
Ce	2.12434	4.1629	5.29638
Ce	5.27906	2.05412	5.29564
Ce	4.31754	3.72131	8.51118
Ce	0.88369	2.08556	8.90447
Ce	1.1619	5.83082	8.51299
Ce	6.71327	0.11221	12.02159
Ce	-0.12412	3.8363	12.04591
Ce	3.08838	1.95394	12.02016
Ce	10.17237	5.92252	1.78864
Ce	3.16308	9.93385	1.76274
Ce	6.54559	7.77093	1.78036
Ce	2.14798	11.70341	4.88771
Ce	5.53481	10.0602	5.29656
Ce	8.68961	7.9492	5.29431
Ce	7.731	9.61763	8.51023
Ce	4.29753	7.98193	8.90902
Ce	4.57582	11.72856	8.5107
Ce	10.12755	6.00744	12.02081
Ce	3.28527	9.73613	12.04371
Ce	6.50377	7.85061	12.02215
Ce	3.34923	5.93135	1.78014
Ce	-3.64617	9.93576	1.75699
Ce	-0.27308	7.76548	1.78444
Ce	-4.66903	11.69938	4.88509
Ce	-1.28124	10.06126	5.29677
Ce	1.87522	7.95277	5.2974
Ce	0.91181	9.61635	8.51164
Ce	-2.52168	7.98247	8.90918
Ce	-2.24211	11.72934	8.51056
Ce	3.30567	6.0085	12.02097
Ce	-3.53295	9.73943	12.04431
Ce	-0.31878	7.84591	12.01888
Ce	13.57489	0.03366	1.78087
Ce	6.57502	4.04124	1.76072
Ce	9.94956	1.87252	1.77876

Ce	5.55169	5.80576	4.88388
Ce	8.93704	4.16254	5.2959
Ce	12.09435	2.05174	5.29534
Ce	11.13602	3.7216	8.51328
Ce	7.70245	2.08633	8.90917
Ce	7.98066	5.83174	8.50914
Ce	13.52941	0.11172	12.02167
Ce	6.68595	3.83651	12.04471
Ce	9.90925	1.95827	12.02399
O	4.28716	3.82957	1.23854
O	4.48261	0.01065	1.23241
O	0.89282	2.07097	1.17686
O	3.17143	2.22481	4.19409
O	-0.08059	3.74921	4.18533
O	-1.30846	5.88803	2.679
O	-2.387	4.20372	6.19987
O	6.4344	0.17991	4.19547
O	4.08635	0.07574	6.19962
O	-0.29577	4.13383	9.61803
O	-1.06012	1.91175	7.60511
O	2.0081	3.67978	7.60522
O	0.93638	1.99399	11.1293
O	3.26362	5.65085	9.6135
O	3.41872	1.81249	9.60859
O	-1.26713	5.80513	12.62244
O	5.36511	1.96864	12.56428
O	2.15284	4.0459	12.57427
O	7.70765	9.72384	1.23542
O	7.89824	5.90983	1.24217
O	4.30564	7.96568	1.1738
O	6.57947	8.12278	4.19405
O	3.33234	9.6477	4.18179
O	2.10488	11.78354	2.66656
O	1.0299	10.10368	6.20269
O	9.83814	6.07213	4.19513
O	7.49683	5.97226	6.20017
O	3.11437	10.02983	9.62376
O	2.35392	7.80883	7.6087
O	5.42072	9.57474	7.60605
O	4.35253	7.88998	11.13478
O	6.67832	11.54646	9.60923
O	6.83502	7.70832	9.60965
O	2.15141	11.70874	12.63208
O	8.77789	7.8679	12.56665
O	5.56941	9.94403	12.56812
O	0.88357	9.72428	1.24781
O	1.07545	5.90396	1.23292
O	-2.51583	7.96053	1.17216

O	-0.23071	8.12967	4.20079
O	-3.48212	9.64584	4.18045
O	-4.71612	11.77744	2.66462
O	-5.79036	10.09883	6.19679
O	3.0273	6.07416	4.19306
O	0.68408	5.9704	6.20031
O	-3.70336	10.03338	9.62191
O	-4.46181	7.80722	7.6025
O	-1.39772	9.57269	7.60557
O	-2.47186	7.89359	11.1352
O	-0.13859	11.5473	9.61161
O	0.00931	7.70378	9.60965
O	-4.67319	11.70887	12.63368
O	1.95683	7.87189	12.55847
O	-1.25389	9.94748	12.56614
O	11.11193	3.8272	1.2435
O	11.30047	0.00761	1.23523
O	7.71055	2.06749	1.16801
O	9.9848	2.22718	4.19726
O	6.73848	3.75149	4.18003
O	5.50483	5.88292	2.66226
O	4.43321	4.20447	6.19816
O	13.25042	0.17862	4.19451
O	10.90438	0.07414	6.19935
O	6.51988	4.13432	9.62306
O	5.75966	1.91326	7.60687
O	8.82489	3.68024	7.60822
O	7.75885	1.99453	11.13474
O	10.0845	5.65073	9.612
O	10.23972	1.81253	9.61261
O	5.55253	5.80966	12.62957
O	12.18595	1.96512	12.5715
O	8.96807	4.05211	12.56988

NF3

Periodic vectors

13.8335521878410006 0.0000000000000000
6.8960907198511201 11.9443795003864004

XYZ coordinates

Ce	8.98862526	3.80242591	4.28566862
Ce	5.7039729	5.63556425	4.31682648
Ce	5.67658597	1.94412874	4.27832604
Ce	1.19085553	1.63734267	10.86986657
Ce	5.46579629	1.80691794	14.11638059
Ce	6.93008053	3.79185218	7.37828957
Ce	10.07099831	5.96139673	7.7044934
Ce	3.12316984	1.59366999	7.71722817
Ce	8.11397643	5.95779674	10.95582363
Ce	2.28435977	3.57914585	14.21777497
Ce	4.3788242	3.85220288	11.27579532
Ce	5.82560715	5.97903055	14.17380591
Ce	19.35344671	9.77461566	4.28566862
Ce	16.06879436	11.607754	4.31682648
Ce	16.04140742	7.91631849	4.27832604
Ce	11.55567699	7.60953242	10.86986657
Ce	15.83061774	7.77910769	14.11638059
Ce	17.29490888	9.76405388	7.37828957
Ce	20.43581976	11.93358648	7.7044934
Ce	13.48799129	7.56585974	7.71722817
Ce	18.47879788	11.92998649	10.95582363
Ce	12.64917433	9.55132366	14.21777497
Ce	14.74364565	9.82439263	11.27579532
Ce	9.29433099	0.00682886	14.17380591
Ce	12.43667062	9.77461566	4.28566862
Ce	9.15201826	11.607754	4.31682648
Ce	9.12463133	7.91631849	4.27832604
Ce	4.63890089	7.60953242	10.86986657
Ce	8.91384165	7.77910769	14.11638059
Ce	10.37813279	9.76405388	7.37828957
Ce	13.51904367	11.93358648	7.7044934
Ce	6.5712152	7.56585974	7.71722817
Ce	11.56202179	11.92998649	10.95582363
Ce	5.73239824	9.55132366	14.21777497
Ce	7.82686956	9.82439263	11.27579532
Ce	2.3775549	0.00682886	14.17380591
Ce	15.90540135	3.80242591	4.28566862
Ce	12.620749	5.63556425	4.31682648
Ce	12.59336206	1.94412874	4.27832604

Ce	8.10763163	1.63734267	10.86986657
Ce	12.38257238	1.80691794	14.11638059
Ce	13.84685663	3.79185218	7.37828957
Ce	16.9877744	5.96139673	7.7044934
Ce	10.03994593	1.59366999	7.71722817
Ce	15.03075252	5.95779674	10.95582363
Ce	9.20113587	3.57914585	14.21777497
Ce	11.29560029	3.85220288	11.27579532
Ce	12.74238325	5.97903055	14.17380591
O	7.98324483	5.91916476	3.75929402
O	4.33027476	3.81921056	3.70593763
O	5.38787294	5.85346879	6.69218539
O	7.77217715	1.99900565	8.5252875
O	6.81210215	3.76349182	5.13186456
O	3.46535207	5.635053	10.03387928
O	5.39008925	1.73038209	6.67619152
O	1.07556098	1.61049292	3.78113794
O	2.39231708	3.79060836	6.65261157
O	7.76554294	5.57285011	8.62355721
O	7.79120278	1.73033667	14.13539154
O	3.49475675	2.00673521	9.99170237
O	15.9209076	3.69318288	11.91189113
O	8.16516274	5.69992876	13.88841991
O	3.44255696	1.83998748	15.20368993
O	5.90759758	5.89210288	11.83747643
O	4.55399498	3.98611049	13.69938613
O	5.78314835	1.8874699	11.81465119
O	18.34805245	11.89135451	3.75929402
O	14.69509621	9.79140031	3.70593763
O	15.75270129	11.82567049	6.69218539
O	18.1369986	7.9711954	8.5252875
O	17.17690977	9.73568157	5.13186456
O	13.83017352	11.60724275	10.03387928
O	15.75491071	7.70257184	6.67619152
O	11.44038243	7.58268267	3.78113794
O	12.75713853	9.76279811	6.65261157
O	18.13037129	11.5450518	8.62355721
O	18.15603807	7.70252642	14.13539154
O	13.8595782	7.97892496	9.99170237
O	12.45217687	9.66537263	11.91189113
O	18.5299842	11.67211851	13.88841991
O	13.80737841	7.81217723	15.20368993
O	16.27241903	11.86429263	11.83747643
O	14.91881644	9.95830024	13.69938613
O	16.1479698	7.85965965	11.81465119
O	11.43129019	11.89135451	3.75929402
O	7.77832012	9.79140031	3.70593763
O	8.83592519	11.82567049	6.69218539

O	11.22022251	7.9711954	8.5252875
O	10.26014751	9.73568157	5.13186456
O	6.91339743	11.60724275	10.03387928
O	8.83813461	7.70257184	6.67619152
O	4.52360634	7.58268267	3.78113794
O	5.84036244	9.76279811	6.65261157
O	11.2135952	11.5450518	8.62355721
O	11.23926198	7.70252642	14.13539154
O	6.94280211	7.97892496	9.99170237
O	19.36895296	9.66537263	11.91189113
O	11.6132081	11.67211851	13.88841991
O	6.89060232	7.81217723	15.20368993
O	9.35564294	11.86429263	11.83747643
O	8.00204034	9.95830024	13.69938613
O	9.23119371	7.85965965	11.81465119
O	14.9000071	5.91916476	3.75929402
O	11.24705085	3.81921056	3.70593763
O	12.30464903	5.85346879	6.69218539
O	14.68895324	1.99900565	8.5252875
O	13.72886441	3.76349182	5.13186456
O	10.38212816	5.635053	10.03387928
O	12.30686535	1.73038209	6.67619152
O	7.99233707	1.61049292	3.78113794
O	9.30909317	3.79060836	6.65261157
O	14.68231903	5.57285011	8.62355721
O	14.70799271	1.73033667	14.13539154
O	10.41152595	2.00672326	9.99170237
O	9.00413151	3.69318288	11.91189113
O	15.08193884	5.69992876	13.88841991
O	10.35933305	1.83998748	15.20368993
O	12.82437367	5.89210288	11.83747643
O	11.47077108	3.98611049	13.69938613
O	12.69992444	1.8874699	11.81465119

NF4

Periodic vectors

14.065448000 0.000000000
-7.036825170 12.188138719

XYZ coordinates

Ce	6.93441	0.03851	1.66448
Ce	0.07666	3.57304	1.63492
Ce	3.40623	1.15037	1.5852
Ce	-1.18022	5.43621	4.54678
Ce	2.35833	3.86727	4.92038
Ce	5.4792	1.67795	4.75776
Ce	4.51344	3.35123	8.12188
Ce	0.92415	1.79725	8.33305
Ce	1.33161	5.64768	7.9579
Ce	3.8255	5.43521	11.21419
Ce	-0.06065	3.81685	11.24284
Ce	3.02905	1.82685	11.30027
Ce	10.44871	6.13258	1.66448
Ce	3.59097	9.66711	1.63492
Ce	6.92055	7.24443	1.5852
Ce	2.33409	11.53028	4.54678
Ce	5.87264	9.96134	4.92038
Ce	8.99351	7.77202	4.75776
Ce	8.02775	9.4453	8.12188
Ce	4.43846	7.89132	8.33305
Ce	4.84592	11.74175	7.9579
Ce	7.3398	11.52928	11.21419
Ce	3.45366	9.91092	11.24284
Ce	6.54338	7.92092	11.30027
Ce	3.416	6.13258	1.66448
Ce	-3.44175	9.66711	1.63492
Ce	-0.11218	7.24443	1.5852
Ce	-4.69863	11.53028	4.54678
Ce	-1.16008	9.96134	4.92038
Ce	1.96079	7.77202	4.75776
Ce	0.99503	9.4453	8.12188
Ce	-2.59427	7.89132	8.33305
Ce	-2.18681	11.74175	7.9579
Ce	0.30709	11.52928	11.21419
Ce	-3.57906	9.91092	11.24284
Ce	-0.48936	7.92092	11.30027
Ce	13.96712	0.03851	1.66448
Ce	7.10938	3.57304	1.63492
Ce	10.43895	1.15037	1.5852

Ce	5.85251	5.43621	4.54678
Ce	9.39105	3.86727	4.92038
Ce	12.51193	1.67795	4.75776
Ce	11.54617	3.35123	8.12188
Ce	7.95687	1.79725	8.33305
Ce	8.36433	5.64768	7.9579
Ce	10.85821	5.43521	11.21419
Ce	6.97207	3.81685	11.24284
Ce	10.06179	1.82685	11.30027
O	5.56548	1.87461	2.13678
O	1.31898	5.42549	0.98079
O	1.28007	1.75056	0.84876
O	3.15794	1.68291	3.8822
O	0.17536	3.51439	3.94234
O	-1.38961	5.35922	2.16794
O	4.68238	3.79926	5.71575
O	3.35763	5.87365	3.98617
O	0.86525	5.73832	5.70801
O	-0.06507	3.93341	8.93728
O	5.95308	1.60101	7.16409
O	2.20442	3.42006	7.17098
O	0.75847	1.65532	10.70895
O	3.56981	5.51179	8.89356
O	3.35919	1.33912	8.99821
O	-1.03807	5.77144	12.02702
O	4.72807	3.32638	10.74397
O	2.16586	3.96506	11.89899
O	9.07979	7.96868	2.13678
O	4.8333	11.51956	0.98079
O	4.79438	7.84463	0.84876
O	6.67225	7.77698	3.8822
O	3.68967	9.60846	3.94234
O	2.1247	11.45329	2.16794
O	8.19669	9.89333	5.71575
O	6.87194	11.96772	3.98617
O	4.37957	11.83239	5.70801
O	3.44924	10.02748	8.93728
O	9.46739	7.69508	7.16409
O	5.71873	9.51413	7.17098
O	4.27278	7.74939	10.70895
O	7.08412	11.60586	8.89356
O	6.8735	7.43319	8.99821
O	2.47624	11.86551	12.02702
O	8.24238	9.42045	10.74397
O	5.68017	10.05912	11.89899
O	2.04707	7.96868	2.13678
O	-2.19943	11.51956	0.98079
O	-2.23834	7.84463	0.84876

O	-0.36047	7.77698	3.8822
O	-3.34305	9.60846	3.94234
O	-4.90802	11.45329	2.16794
O	1.16397	9.89333	5.71575
O	-0.16078	11.96772	3.98617
O	-2.65316	11.83239	5.70801
O	-3.58348	10.02748	8.93728
O	2.43467	7.69508	7.16409
O	-1.31399	9.51413	7.17098
O	-2.75994	7.74939	10.70895
O	0.0514	11.60586	8.89356
O	-0.15922	7.43319	8.99821
O	-4.55648	11.86551	12.02702
O	1.20966	9.42045	10.74397
O	-1.35255	10.05912	11.89899
O	12.5982	1.87461	2.13678
O	8.35171	5.42549	0.98079
O	8.3128	1.75056	0.84876
O	10.19066	1.68291	3.8822
O	7.20808	3.51439	3.94234
O	5.64311	5.35922	2.16794
O	11.71511	3.79926	5.71575
O	10.39036	5.87365	3.98617
O	7.89798	5.73832	5.70801
O	6.96765	3.93341	8.93728
O	12.98581	1.60101	7.16409
O	9.23714	3.42006	7.17098
O	7.7912	1.65532	10.70895
O	10.60254	5.51179	8.89356
O	10.39192	1.33912	8.99821
O	5.99466	5.77143	12.02702
O	11.76079	3.32638	10.74397
O	9.19859	3.96506	11.89899