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Supporting information for article:

***DFT2FEFFIT*: a DFT-based structural toolkit to analyze EXAFS spectra**

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S1. DFT calculation

DFT computations were performed in the Vienna Ab-initio Simulation Package (VASP) software (Kresse, 1995; Kresse & Furthmuller, 1996). The projector augmented wave (PAW) pseudopotentials (Blochl, 1994; Kresse & Joubert, 1999) were used for the core-electron interaction, in combination with a converged energy cutoff of 500 eV for the planewave basis set. The energies and forces were evaluated at the generalized gradient approximation (GGA) with a Perdew-Burke-Ernzerhof (PBE; Perdew *et al.*, 1996) exchange-correlation functional in conjunction with the density-dependent dispersion correction dDsC (Steinmann & Corminboeuf, 2011; Gautier *et al.*, 2015). The Brillouin zone of 2 x 2 x 2 supercells with stoichiometry $\text{Ca}_{80}\text{P}_{48}\text{O}_{192}\text{F}_{16}$ (FAp has two formula units in the primitive cell) and cell vector lengths of about 18.8 Å and 13.7 Å for in-plane and out-of-plane directions was probed at the Gamma point. A Fermi-smearing of 0.026 eV (~300 K) was applied, but had no impact on the electronic energy for this insulating material with a band gap of at least 4 eV. During the self-consistent field procedure, the wave functions were optimized to an energy-change below 10^{-6} eV. The numerical settings for the fast Fourier transformation grids was set to “accurate” and the real-space projector operators were determined via the recommended automatic optimization scheme. For geometry optimizations all atoms and the unit cell were fully relaxed until the maximum force was below 0.05 eV/Å. The atomic Hirshfeld charges, which are known to depend little on the electronic structure and the basis set and are well suited for assessing charge-transfers (Gonthier *et al.*, 2012), have been taken from the standard output of the dDsC dispersion correction. The maximum error in the interatomic distances of FAp calculated with VASP relative to the diffraction values (Hughes *et al.*, 1989) is 1.15% (Manceau *et al.*, 2024). The starting configurations of the substitutional models are produced by replacing one element by another in the FAp structure. No symmetry constraints were applied, VASP guesses an initial symmetry based on the initial coordinates and unit cell.

S2. Input script and best-fit parameters of the Ce2-Si-close model

Input :

Ce-EXAFS_Durango_RT.chi

22

2

2.5 10.4

0.9

1
-2.5 -0.5 0.3
1; F; 2.379; chip0001.dat;FEFF;1;0.06; 0.04; 0.13; 2
2; O; 2.415; chip0002.dat; FEFF; 1; 0.06; 0.04; 0.13; -1
3; O; 2.416; chip0003.dat; FEFF; 1; 0.06; 0.04; 0.13; 2
4; O; 2.436; chip0004.dat; FEFF; 1; 0.06; 0.04; 0.13; 2
5; O; 2.437; chip0005.dat; FEFF; 1; 0.06; 0.04; 0.13; 2
6; O; 2.487; chip0006.dat; FEFF; 1; 0.06; 0.04; 0.13; 2
7; O; 2.754; chip0007.dat; FEFF; 1; 0.06; 0.04; 0.13; 2
8; Si; 3.095; chip0008.dat; FEFF; 1; 0.06; 0.04; 0.13; -1
11; P; 3.197; chip0011.dat; FEFF; 1; 0.06; 0.04; 0.13; 8
13; P; 3.616; chip0013.dat; FEFF; 1; 0.06; 0.04; 0.13; -1
14; 2P; 3.774; chip0014.dat; FEFF; 1; 0.06; 0.04; 0.13; 13
15; Ca; 3.967; chip0015.dat; FEFF; 1; 0.06; 0.04; 0.13; -1
16; Ca; 4.010; chip0016.dat; FEFF; 1; 0.06; 0.04; 0.13; 15
20; Ca; 4.066; chip0020.dat; FEFF; 1; 0.06; 0.04; 0.13; 15
21; Ca; 4.068; chip0021.dat; FEFF; 1; 0.06; 0.04; 0.13; 15
24; Ca; 4.100; chip0024.dat; FEFF; 1; 0.06; 0.04; 0.13; 15
25; Ca; 4.101; chip0025.dat; FEFF; 1; 0.06; 0.04; 0.13; 15
26; Ca; 4.131; chip0026.dat; FEFF; 1; 0.06; 0.04; 0.13; 15
27; Ca; 4.133; chip0027.dat; FEFF; 1; 0.06; 0.04; 0.13; 15
28; Ca; 4.144; chip0028.dat; FEFF; 1; 0.06; 0.04; 0.13; 15
29; Ca; 4.148; chip0029.dat; FEFF; 1; 0.06; 0.04; 0.13; 15
30; MS; 4.000; Ce2-Si-close_MS.chi; 2C; 1; 0.10; 0.08; 0.17; -1

Best-fit parameters:

$\Delta E = -1.0$ eV; $\sigma(\text{O},\text{F}) = 0.12$ Å; $\sigma(\text{Si},\text{P1}) = 0.07$ Å; $\sigma(\text{P2}) = 0.12$ Å; $\sigma(\text{Ca}) = 0.11$ Å; ; $\sigma(\text{MS}) = 0.17$ Å; $NSS = 0.10$

The σ values of the cation shells at 8-12 K are: $\sigma(\text{Si},\text{P1}) = 0.04$ Å; $\sigma(\text{P2}) = 0.09$ Å; $\sigma(\text{Ca}) = 0.08$ Å (Manceau *et al.*, 2024).

S3. Input script and best-fit parameters of the Ce2-F model

Input :

Ce-EXAFS_Durango_RT.chi

24

2

2.5 10.4

0.9

1

-2.5 -0.5 0.3

1; F;2.31;chip0001.dat;FEFF;1;0.06; 0.04; 0.13; 2
2; O;2.31;chip0002.dat;FEFF;1; 0.06;0.04; 0.13; -1
3; O;2.31;chip0003.dat;FEFF;1; 0.06;0.04; 0.13; 2
4; O;2.31;chip0004.dat;FEFF;1; 0.06;0.04; 0.13; 2
5; O;2.31;chip0005.dat;FEFF;1; 0.06;0.04; 0.13; 2
6; O;2.31;chip0006.dat;FEFF;1; 0.06;0.04; 0.13; 2
7; O;2.31;chip0007.dat;FEFF;1; 0.06;0.04; 0.13; 2
8; O;2.31;chip0008.dat;FEFF;1; 0.06;0.04; 0.13; 2
10; P;2.31;chip0010.dat;FEFF;1; 0.06;0.04; 0.13; -1

11; P;2.31;chip0011.dat;FEFF;1; 0.06; 0.04; 0.13;10
 14; P;2.31;chip0014.dat;FEFF;1; 0.06; 0.04; 0.13; -1
 17; P;2.31;chip0017.dat;FEFF;1;0.06; 0.04; 0.13; 14
 18; P;2.31;chip0018.dat;FEFF;1;0.06; 0.04; 0.13; 14
 13; Ca;2.31;chip0013.dat;FEFF;1;0.06; 0.04; 0.15; -1
 16; Ca;2.31;chip0016.dat;FEFF;1;0.06; 0.04; 0.15; 13
 19; Ca;2.31;chip0019.dat;FEFF;1;0.06; 0.04; 0.15; 13
 20; Ca;2.31;chip0020.dat;FEFF;1;0.06; 0.04; 0.15; 13
 21; Ca;2.31;chip0021.dat;FEFF;1;0.06; 0.04; 0.15; 13
 23; Ca;2.31;chip0023.dat;FEFF;1;0.06; 0.04; 0.15; 13
 24; Ca;2.31;chip0024.dat;FEFF;1;0.06; 0.04; 0.15; 13
 27; Ca;2.31;chip0027.dat;FEFF;1;0.06; 0.04; 0.15; 13
 28; Ca;2.31;chip0028.dat;FEFF;1;0.06; 0.04; 0.15; 13
 29; Ca;2.31;chip0029.dat;FEFF;1;0.06; 0.04; 0.15; 13
 30; F;2.31;Ce2_F_interstitiel_MS.dat;2C;1;0.10; 0.08; 0.17; -1

Best-fit parameters:

$\Delta E = -2.5$ eV; $\sigma(\text{O,F}) = 0.13$ Å; $\sigma(\text{P1}) = 0.08$ Å; $\sigma(\text{P2}) = 0.13$ Å; $\sigma(\text{Ca}) = 0.12$ Å; ; $\sigma(\text{MS}) = 0.17$ Å;
 NSS = 0.31

S4. Input script and best-fit parameters of the 2Ce2-Vac model

The amplitude of the Durango spectrum was multiplied by two to fit the DFT spectra at the Ce2_1-Vac and Ce2_2-Vac sites, and afterward the experimental and optimized spectra were divided by two.

Input:

```
Ce-EXAFS_Durango_RTx2.chi
44
2
2.5 10.4
0.9
1
-2.5 -0.5 0.3
#Ce2-1-Vac site
1; F;2.31;chip0001_1.dat;FEFF;1;0.06; 0.04; 0.13; 2
2; O;2.31;chip0002_1.dat;FEFF;1; 0.06;0.04; 0.13; -1
3; O;2.31;chip0003_1.dat;FEFF;1; 0.06;0.04; 0.13; 2
4; O;2.31;chip0004_1.dat;FEFF;1; 0.06;0.04; 0.13; 2
5; O;2.31;chip0005_1.dat;FEFF;1; 0.06;0.04; 0.13; 2
6; O;2.31;chip0006_1.dat;FEFF;1; 0.06;0.04; 0.13; 2
7; O;2.31;chip0007_1.dat;FEFF;1; 0.06;0.04; 0.13; 2
8; P;2.31;chip0008_1.dat;FEFF;1; 0.06;0.04; 0.13; -1
9; P;2.31;chip0009_1.dat;FEFF;1; 0.06; 0.04; 0.13;8
13; P;2.31;chip0013_1.dat;FEFF;1; 0.06; 0.04; 0.13; -1
14; P;2.31;chip0014_1.dat;FEFF;1;0.06; 0.04; 0.13; 13
15; P;2.31;chip0015_1.dat;FEFF;1;0.06; 0.04; 0.13; 13
19; Ca;2.31;chip0019_1.dat;FEFF;1;0.06; 0.04; 0.15; -1
20; Ca;2.31;chip0020_1.dat;FEFF;1;0.06; 0.04; 0.15; 19
21; Ce2;2.31;chip0021_1.dat;FEFF;1;0.06; 0.04; 0.15; -1
23; Ca;2.31;chip0023_1.dat;FEFF;1;0.06; 0.04; 0.15; 19
```

24; Ca;2.31;chip0024_1.dat;FEFF;1;0.06; 0.04; 0.15; 19
 25; Ca;2.31;chip0025_1.dat;FEFF;1;0.06; 0.04; 0.15; 19
 26; Ca;2.31;chip0026_1.dat;FEFF;1;0.06; 0.04; 0.15; 19
 28; Ca;2.31;chip0028_1.dat;FEFF;1;0.06; 0.04; 0.15; 19
 29; Ca;2.31;chip0029_1.dat;FEFF;1;0.06; 0.04; 0.15; 19
 30; MS;2.31;Ce2_1_Vac_Together_MS.chi;2C;1;0.10; 0.08; 0.17; -1
 #Ce2-2-Vac site
 31; F;2.31;chip0001_2.dat;FEFF;1;0.06; 0.04; 0.13; 2
 32; O;2.31;chip0002_2.dat;FEFF;1; 0.06;0.04; 0.13; 2
 33; O;2.31;chip0003_2.dat;FEFF;1; 0.06;0.04; 0.13; 2
 34; O;2.31;chip0004_2.dat;FEFF;1; 0.06;0.04; 0.13; 2
 35; O;2.31;chip0005_2.dat;FEFF;1; 0.06;0.04; 0.13; 2
 36; O;2.31;chip0006_2.dat;FEFF;1; 0.06;0.04; 0.13; 2
 37; O;2.31;chip0007_2.dat;FEFF;1; 0.06;0.04; 0.13; 2
 38; P;2.31;chip0010_2.dat;FEFF;1; 0.06;0.04; 0.13; 8
 39; P;2.31;chip0011_2.dat;FEFF;1; 0.06; 0.04; 0.13;8
 40; P;2.31;chip0013_2.dat;FEFF;1; 0.06; 0.04; 0.13; 13
 41; P;2.31;chip0014_2.dat;FEFF;1;0.06; 0.04; 0.13; 13
 42; P;2.31;chip0015_2.dat;FEFF;1;0.06; 0.04; 0.13; 13
 43; Ca;2.31;chip0016_2.dat;FEFF;1;0.06; 0.04; 0.15; 19
 44; Ca;2.31;chip0017_2.dat;FEFF;1;0.06; 0.04; 0.15; 19
 45; Ca;2.31;chip0018_2.dat;FEFF;1;0.06; 0.04; 0.15; 19
 46; Ca;2.31;chip0019_2.dat;FEFF;1;0.06; 0.04; 0.15; 19
 47; Ce1;2.31;chip0021_2.dat;FEFF;1;0.06; 0.04; 0.15; 21
 48; Ca;2.31;chip0026_2.dat;FEFF;1;0.06; 0.04; 0.15; 19
 49; Ca;2.31;chip0027_2.dat;FEFF;1;0.06; 0.04; 0.15; 19
 50; Ca;2.31;chip0028_2.dat;FEFF;1;0.06; 0.04; 0.15; 19
 51; Ca;2.31;chip0029_2.dat;FEFF;1;0.06; 0.04; 0.15; 19
 52; MS;2.31;Ce2_2_Vac_Together_MS.chi;2C;1;0.10; 0.08; 0.17; 30

Best-fit parameters:

$\Delta E = -1.3$ eV; $\sigma(\text{O,F}) = 0.05$ Å; $\sigma(\text{P1}) = 0.04$ Å; $\sigma(\text{P2}) = 0.08$ Å; $\sigma(\text{Ca}) = 0.07$ Å; ; $\sigma(\text{MS}) = 0.17$ Å;
 $NSS = 0.17$

S5. References

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S6. EXAFS spectrum (Ce-EXAFS_Durango_RT.chi)

2.0000	0.033285
2.0500	-0.0056294
2.1000	-0.063230
2.1500	-0.10729
2.2000	-0.13473
2.2500	-0.15114
2.3000	-0.15464
2.3500	-0.15564
2.4000	-0.14836
2.4500	-0.13583
2.5000	-0.11378
2.5500	-0.087390
2.6000	-0.052464
2.6500	-0.011952
2.7000	0.024822
2.7500	0.057343
2.8000	0.080193
2.8500	0.098267
2.9000	0.10792
2.9500	0.11015
3.0000	0.10162
3.0500	0.087279
3.1000	0.073539
3.1500	0.052451
3.2000	0.037923
3.2500	0.024309
3.3000	0.019305
3.3500	0.015608
3.4000	0.013077
3.4500	0.012445
3.5000	0.0076357
3.5500	0.0012066
3.6000	-0.0064417
3.6500	-0.017532
3.7000	-0.028536
3.7500	-0.037126
3.8000	-0.043871
3.8500	-0.048288
3.9000	-0.048011
3.9500	-0.047283
4.0000	-0.045498
4.0500	-0.044836
4.1000	-0.039719
4.1500	-0.034825
4.2000	-0.024371
4.2500	-0.011284
4.3000	0.0011470
4.3500	0.010359
4.4000	0.020198

4.4500	0.026280
4.5000	0.027212
4.5500	0.027500
4.6000	0.026110
4.6500	0.022123
4.7000	0.017449
4.7500	0.013199
4.8000	0.010161
4.8500	0.0062488
4.9000	0.0027761
4.9500	0.00062829
5.0000	0.00065193
5.0500	0.0018544
5.1000	0.0012388
5.1500	0.0054323
5.2000	0.0087760
5.2500	0.010786
5.3000	0.011342
5.3500	0.0094710
5.4000	0.0063844
5.4500	-0.00050645
5.5000	-0.0033045
5.5500	-0.0057661
5.6000	-0.0051372
5.6500	-0.0091065
5.7000	-0.012307
5.7500	-0.017990
5.8000	-0.017328
5.8500	-0.016017
5.9000	-0.011794
5.9500	-0.014823
6.0000	-0.014039
6.0500	-0.011419
6.1000	-0.0075582
6.1500	-0.00086814
6.2000	0.0060930
6.2500	0.0098138
6.3000	0.012384
6.3500	0.013952
6.4000	0.014752
6.4500	0.013128
6.5000	0.010026
6.5500	0.0084722
6.6000	0.0056942
6.6500	0.00031908
6.7000	-0.0051293
6.7500	-0.0049745
6.8000	-0.0030537
6.8500	-0.0021290
6.9000	-0.0022931

6.9500 -0.0019634
7.0000 -0.0010604
7.0500 -0.00088457
7.1000 0.0010552
7.1500 0.0013429
7.2000 0.00062010
7.2500 0.00053089
7.3000 -0.0028961
7.3500 -0.0037367
7.4000 -0.0028782
7.4500 -0.0051570
7.5000 -0.0035957
7.5500 -0.0024387
7.6000 -0.00025628
7.6500 -0.00041177
7.7000 -0.00082858
7.7500 0.0021290
7.8000 0.0026348
7.8500 0.0047353
7.9000 0.0033215
7.9500 0.0036446
8.0000 0.0029286
8.0500 0.0025423
8.1000 0.00099688
8.1500 0.0020861
8.2000 -0.00078354
8.2500 -0.0018291
8.3000 -0.0023871
8.3500 -0.0012933
8.4000 -0.0015607
8.4500 -0.00083020
8.5000 -0.00079647
8.5500 -0.00045056
8.6000 -0.00026179
8.6500 -0.00021707
8.7000 -0.00041447
8.7500 -0.00056862
8.8000 0.00065174
8.8500 -0.00058880
8.9000 -0.00033076
8.9500 -0.0012026
9.0000 -0.0023989
9.0500 -0.0022052
9.1000 -0.0016627
9.1500 -0.00050149
9.2000 -0.0026013
9.2500 -0.0014177
9.3000 -0.00092885
9.3500 -0.00040318
9.4000 0.00059581

9.4500 0.0017088
 9.5000 0.0011485
 9.5500 0.0016593
 9.6000 0.0023186
 9.6500 0.0021849
 9.7000 0.0027773
 9.7500 0.0029719
 9.8000 0.0028724
 9.8500 0.0021606
 9.9000 0.0014000
 9.9500 -0.00012312
 10.000 0.00036067
 10.050 -0.00043315
 10.100 0.00054729
 10.150 0.00031970
 10.200 -0.0023175
 10.250 -0.0018420
 10.300 -0.0018910
 10.350 -0.0028566
 10.400 -0.0027410
 10.450 -0.0013883

S7. Cartesian coordinates of the DFT models ($a = 100 \text{ \AA}$, $b = 100 \text{ \AA}$, $c = 100 \text{ \AA}$)

S7.1. Ce2-Si-close

58	5.734951401	10.098389649	5.142576935
14	8.283720557	8.342271684	5.144817405
20	9.370090676	5.424408519	3.448190122
20	9.376116308	5.424321125	6.826188073
20	5.958904535	6.095079503	5.145518040
20	4.687826819	2.698758031	13.750127248
20	4.693408561	2.713379275	6.876911998
20	14.086877586	2.719733768	13.755360374
20	14.078150039	2.725585789	6.871931734
20	-0.004483200	10.854971840	13.754304664
20	-0.055058312	10.868976580	6.878993205
20	9.401377178	10.860903145	13.756694287
20	9.397537895	10.785581731	6.854300521
20	0.014423557	5.426747556	6.855233109
20	-0.002612375	5.427625894	13.731330630
20	9.392324608	5.425238117	13.738868836
20	-4.703039008	13.585914353	6.853416076
20	-4.701550119	13.570243142	13.731485624
20	4.693974238	13.627197860	6.872893959
20	4.679385812	13.595096052	13.718583764
20	8.208381147	1.969455574	1.698607485
20	8.207820740	1.970717912	8.587511429
20	17.598283938	1.985559755	1.700613090
20	17.598676748	1.986564493	8.585190103
20	3.502918287	10.137168770	1.666610328
20	3.503040495	10.139490917	8.620606575

20	12.895954836	10.115763145	1.705875617
20	12.895404060	10.115265608	8.579450927
20	3.592378081	6.131338424	1.715461938
20	3.593729285	6.132664897	8.571564789
20	12.964795464	6.122156302	1.705056385
20	12.965728158	6.122524923	8.581146015
20	-1.125533982	14.271412801	1.699183832
20	-1.126363498	14.271457584	8.586478453
20	8.282877764	14.286484203	1.695790928
20	8.281967283	14.286790469	8.587512083
20	1.111147533	2.012214701	5.142229079
20	1.117317294	2.019883362	12.023269433
20	10.498734633	1.998958040	5.143006728
20	10.502392582	2.020479641	12.023694814
20	-3.608801400	10.146471479	5.143128709
20	-3.584417612	10.155539142	12.023784740
20	5.829724306	10.152704110	12.024821781
20	2.299798305	0.033865710	1.703537355
20	2.299095751	0.033813641	8.582291263
20	11.679769298	0.050821382	1.700912110
20	11.678379959	0.050974113	8.583781769
20	-2.400209037	8.180037214	1.699521768
20	-2.399993643	8.180397856	8.584887906
20	7.005698233	8.159906932	1.706976495
20	7.007247986	8.159851094	8.582361993
20	2.333618655	8.058570229	5.143412125
20	2.394066657	8.105678038	12.024728846
20	11.744980291	8.124179967	5.142734421
20	11.778745130	8.102223051	12.023348118
20	-2.311741993	16.228621618	5.143044527
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S7.3. Ce2_1-Vac

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S7.4. Ce2_2-Vac

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