Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Proton-Polaron and Energy Landscape among Acceptor Doped $ACeO_3$ ($A = Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}$) Proton Conductors for Proton Diffusion

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Table S1: DFT simulated lattice constants among distinct acceptor ($M^{3+} = Y^{3+}, Gd^{3+}, Sc^{3+}, In^{3+}$) doped $ACeO_3$ ($A = Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}$) proton conductors

Composition	DFT Simulated Lattice Constants (Å)														
	x = 0			*x* = 0.125			*x* = 0.25			*x* = 0.375			*x* = 0.50		
	a	b	c	a	b	c	a	b	c	a	b	c	a	b	c
$BaCe_{1-x}Y_xO_{3-\delta}$	6.248	8.796	6.227	6.215	8.748	6.211	6.208	6.212	15.151	6.191	8.673	6.209	6.186	8.652	6.190
$BaCe_{1-x}Gd_xO_{3-\delta}$				6.234	8.773	6.232	6.227	6.227	15.183	6.221	6.221	15.170	6.215	8.702	6.218
$BaCe_{1-x}InxO_{3-\delta}$				6.204	8.682	6.203	6.185	8.651	6.184	6.142	8.629	6.156	6.126	8.615	6.123
$BaCe_{1-x}Sc_xO_{3-\delta}$				6.192	8.597	6.187	6.147	8.580	6.156	6.118	8.562	6.108	6.085	8.540	6.127
$SrCe_{1-x}Y_xO_{3-\delta}$	6.117	8.543	5.956	6.094	8.512	5.937	6.042	8.487	5.922	6.013	8.459	5.904	5.958	8.428	5.883
$SrCe_{1-x}Gd_xO_{3-\delta}$				6.108	8.537	5.944	6.083	8.517	5.913	6.044	8.501	5.872	6.012	8.488	5.845
$SrCe_{1-x}InxO_{3-\delta}$				6.042	8.486	5.901	6.019	8.445	5.875	6.021	8.413	5.839	5.926	8.397	5.808
$SrCe_{1-x}Sc_xO_{3-\delta}$				6.017	8.434	5.872	5.854	8.408	5.840	5.821	8.386	5.811	5.793	8.352	5.783
$CaCe_{1-x}Y_xO_{3-\delta}$	5.694	8.023	5.738	5.670	8.009	5.714	5.651	7.971	5.693	5.620	7.942	5.668	5.591	7.915	5.629
$CaCe_{1-x}Gd_xO_{3-\delta}$				5.686	8.381	5.749	5.668	8.359	5.718	5.636	8.325	5.696	5.614	8.297	5.674
$CaCe_{1-x}InxO_{3-\delta}$				5.634	7.962	5.682	5.607	7.923	5.655	5.579	7.884	5.621	5.543	7.836	5.698
$CaCe_{1-x}Sc_xO_{3-\delta}$				5.602	7.935	5.650	5.582	7.901	5.631	5.540	7.869	5.604	5.516	7.824	5.582
$MgCe_{1-x}Y_xO_{3-\delta}$	5.131	7.486	5.484	5.112	7.455	5.458	5.092	7.428	5.426	5.068	7.397	5.395	5.039	7.371	5.370
$MgCe_{1-x}Gd_xO_{3-\delta}$				5.125	7.463	5.467	5.101	7.440	5.439	5.085	7.419	5.412	5.057	7.382	5.385
$MgCe_{1-x}InxO_{3-\delta}$				5.090	7.429	5.436	5.064	7.403	5.408	5.039	7.381	5.377	5.002	7.354	5.349
$MgCe_{1-x}Sc_xO_{3-\delta}$				5.073	7.407	5.411	5.042	7.375	5.385	5.027	7.342	5.350	5.006	7.319	5.317

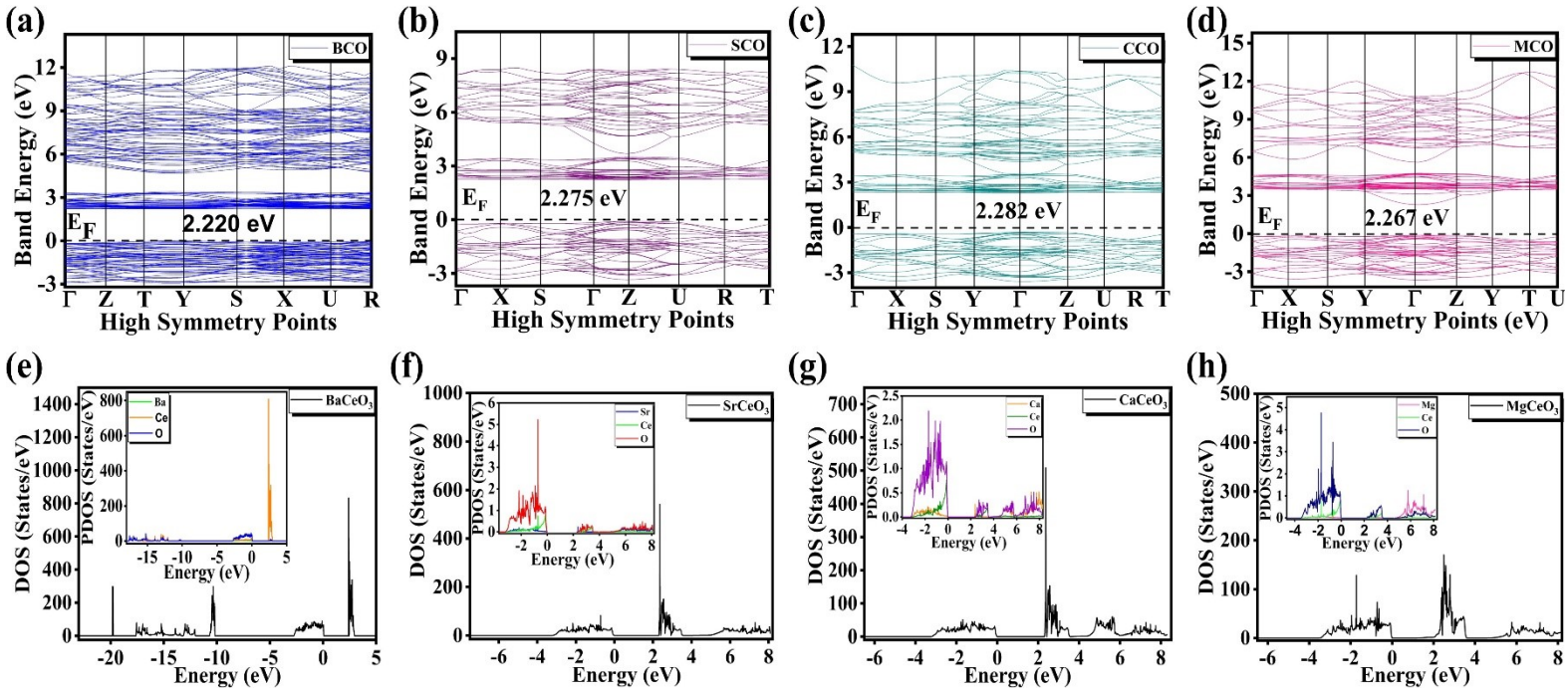

Fig S1: DFT simulated electronic bandstructure and density of states of $ACeO_3$ (A = Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}) proton conductors, (a-d) electronic bandstructure, (e-h) density of states (DOS)

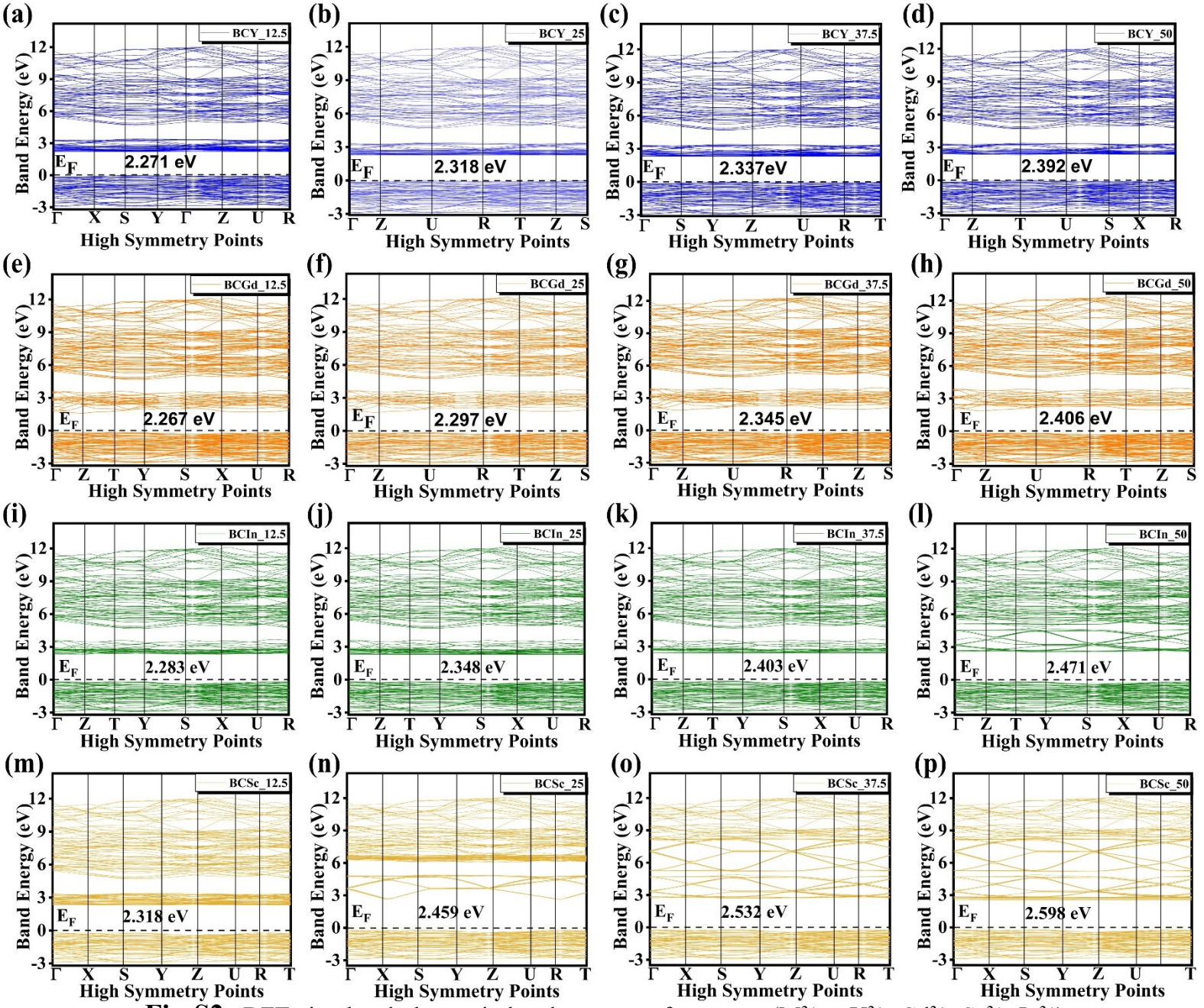

Fig S2: DFT simulated electronic bandstructure of acceptor (M^{3+} = Y^{3+}, Gd^{3+}, Sc^{3+}, In^{3+}) doped $BaCe_{1-x}M_xO_{3-\delta}$ proton conductors at distinct doping concentration (x = 0.125, 0.25, 0.375, 0.50)

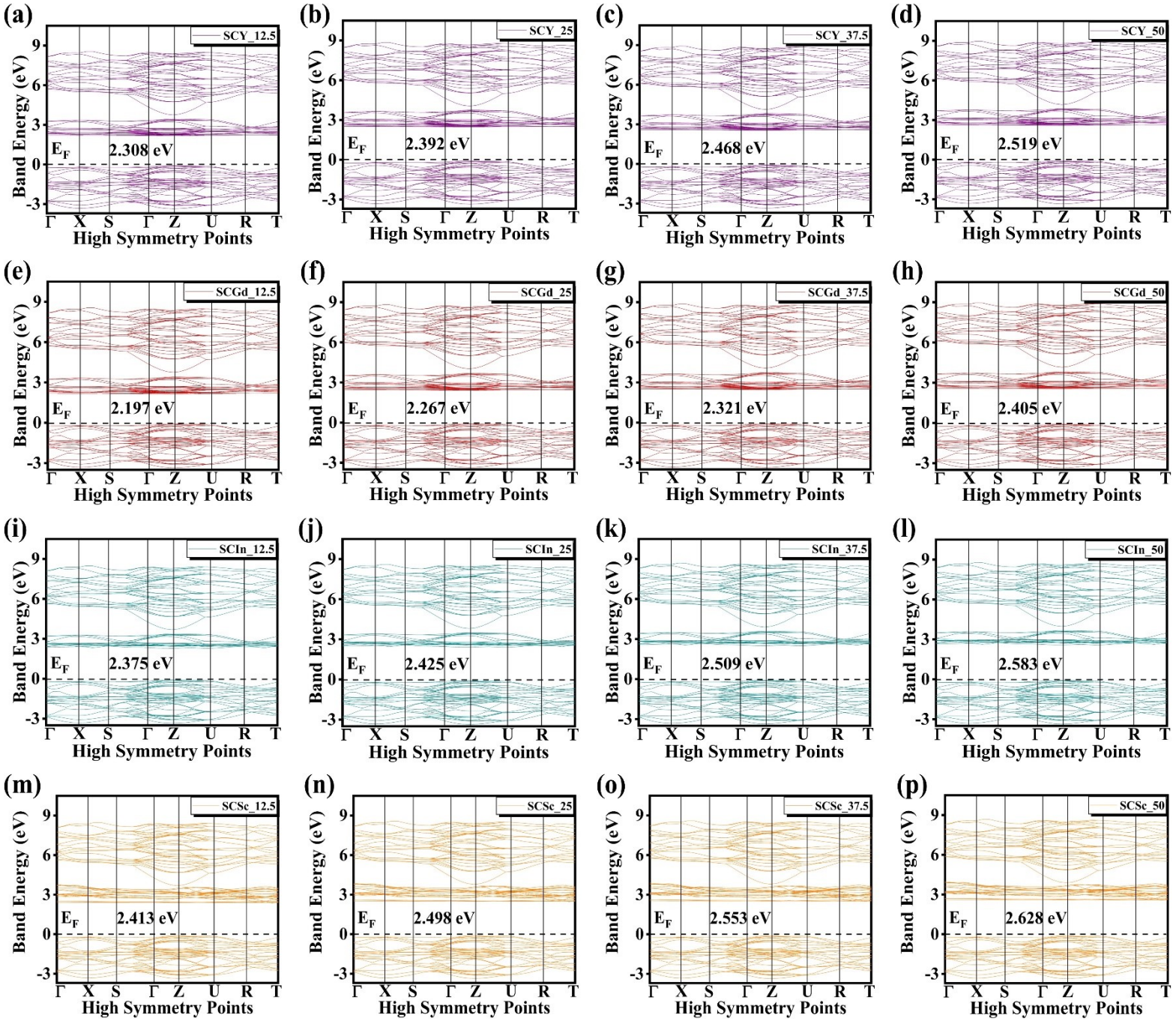

Fig S3: DFT simulated electronic bandstructure of acceptor (M^{3+} = Y^{3+}, Gd^{3+}, Sc^{3+}, In^{3+}) doped $SrCe_{1-x}M_xO_{3-\delta}$ proton conductors at distinct doping concentration (x = 0.125, 0.25, 0.375, 0.50)

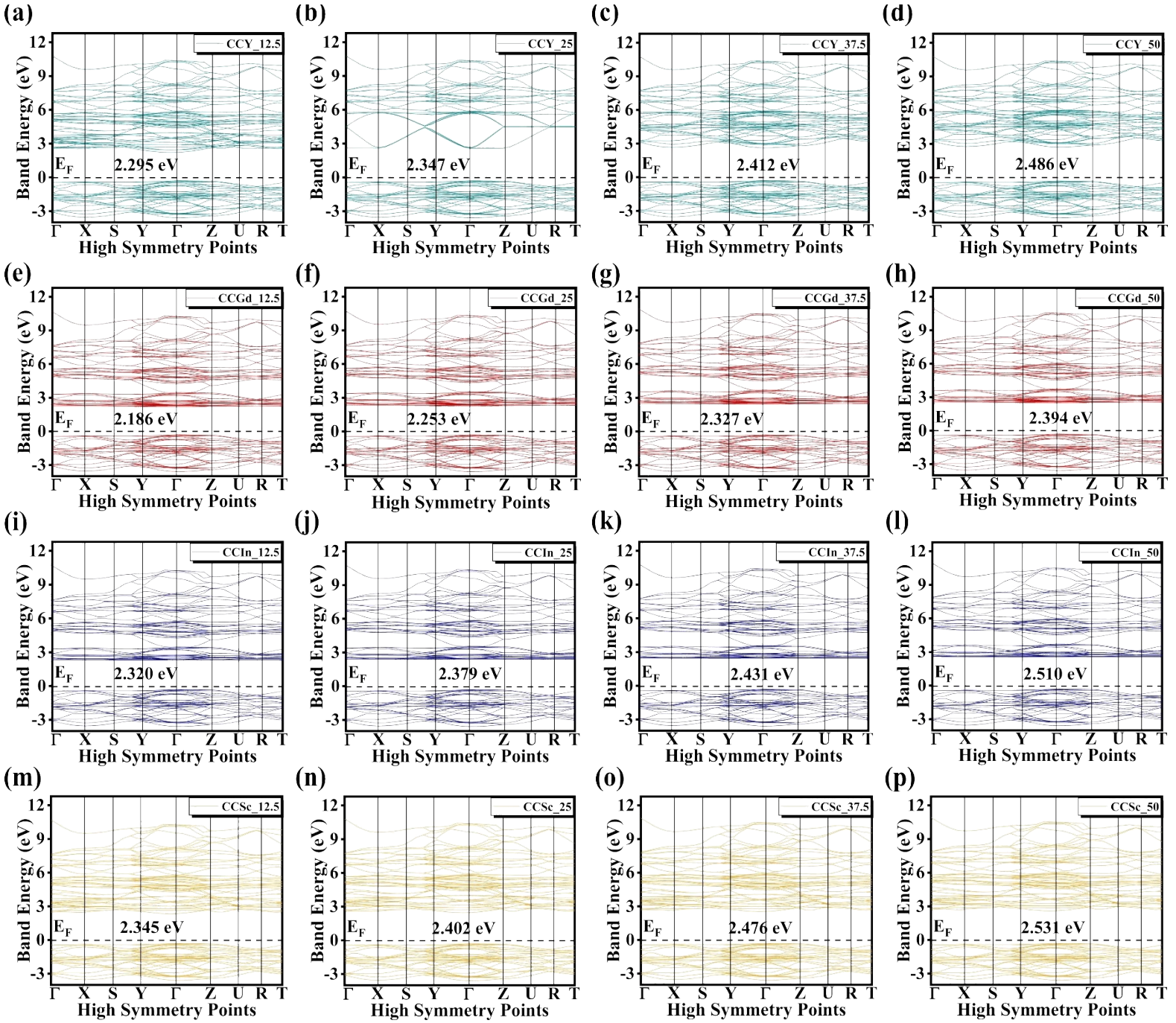

Fig S4: DFT simulated electronic bandstructure of acceptor (M^{3+} = Y^{3+}, Gd^{3+}, Sc^{3+}, In^{3+}) doped $CaCe_{1-x}M_xO_{3-\delta}$ proton conductors at distinct doping concentration (x = 0.125, 0.25, 0.375, 0.50)

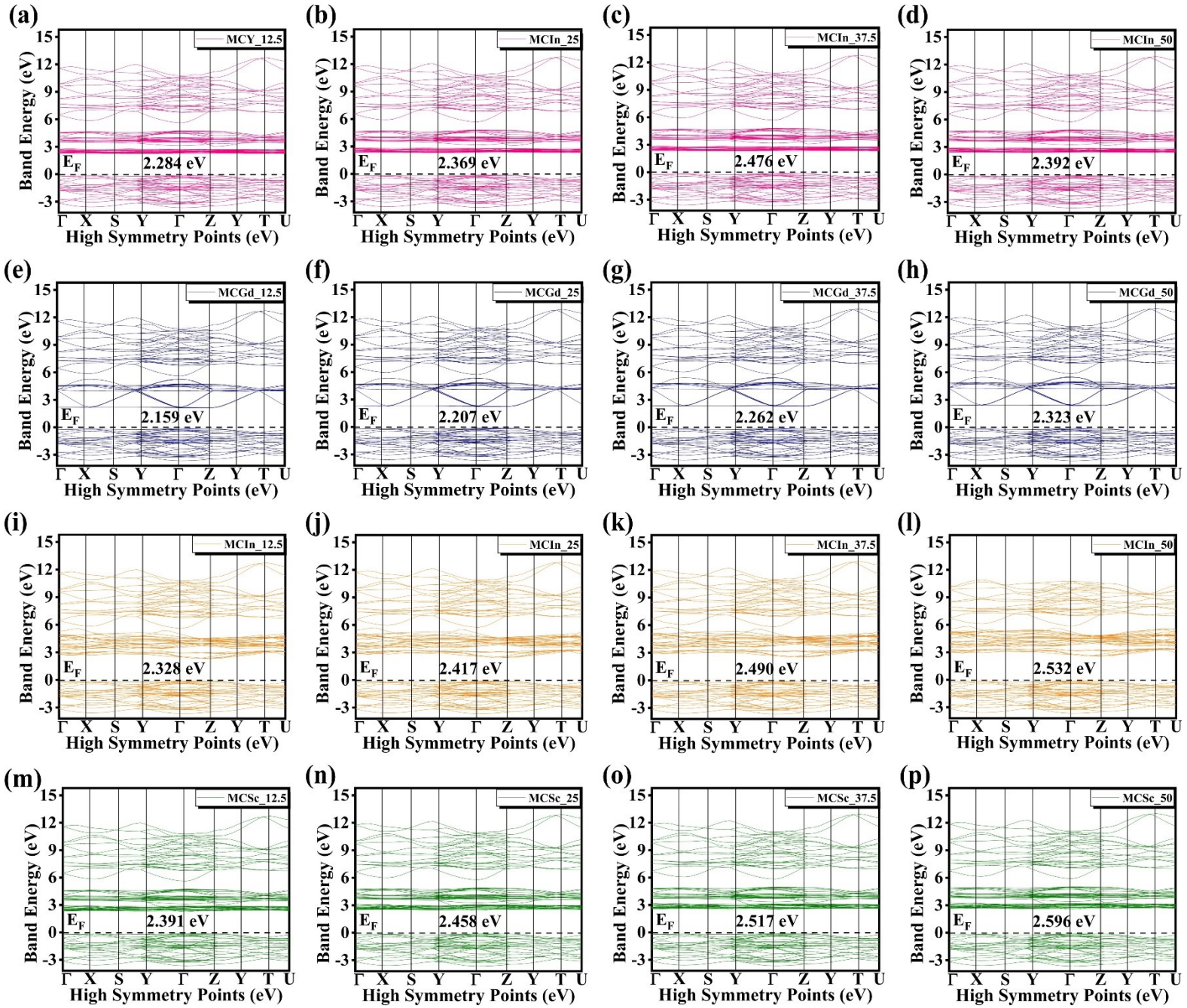

Fig S5: DFT simulated electronic bandstructure of acceptor (M^{3+} = Y^{3+}, Gd^{3+}, Sc^{3+}, In^{3+}) doped $MgCe_{1-x}M_xO_{3-\delta}$ proton conductors at distinct doping concentration (x = 0.125, 0.25, 0.375, 0.50)

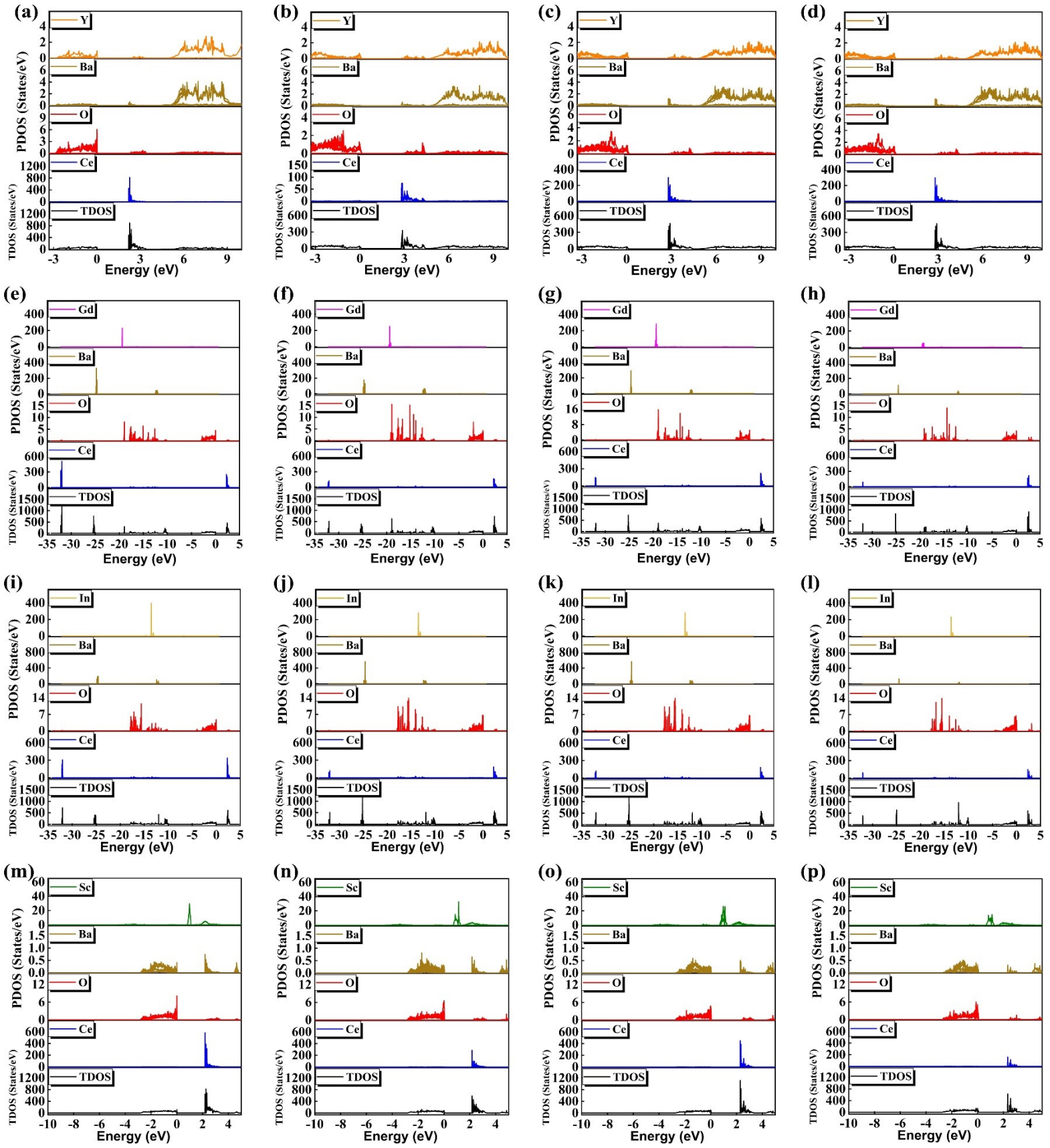

Fig S6: DFT simulated density of states of $BaCe_{1-x}M_xO_{3-\delta}$ ($M = Y^{3+}$, Gd^{3+}, In^{3+}, Sc^{3+}) corresponding to distinct doping concentration (x = 0.125, 0.25, 0.375, 0.5)

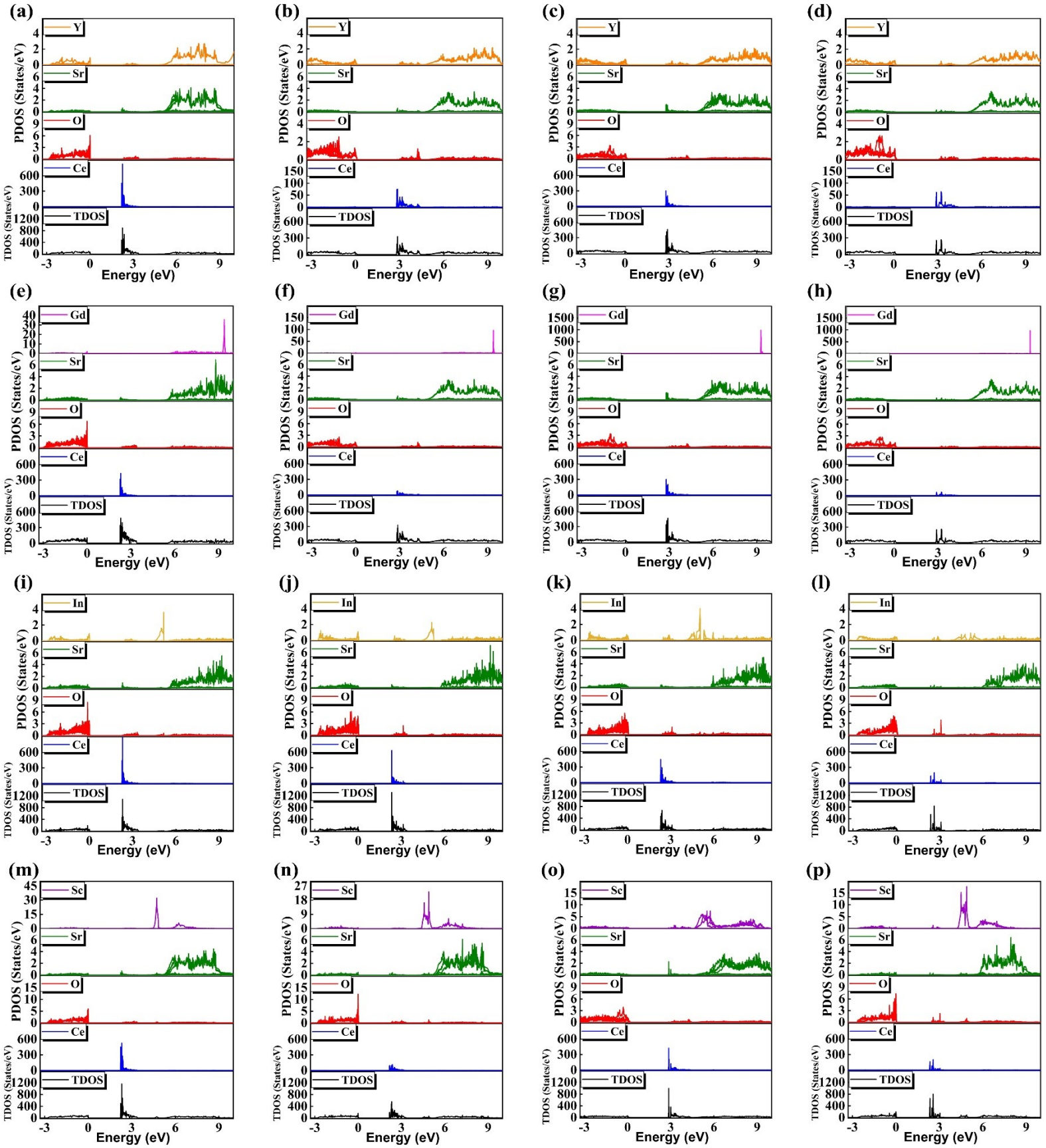

Fig S7: DFT simulated density of states of $SrCe_{1-x}M_xO_{3-\delta}$ ($M = Y^{3+}$, Gd^{3+}, In^{3+}, Sc^{3+}) corresponding to distinct doping concentration (x = 0.125, 0.25, 0.375, 0.5)

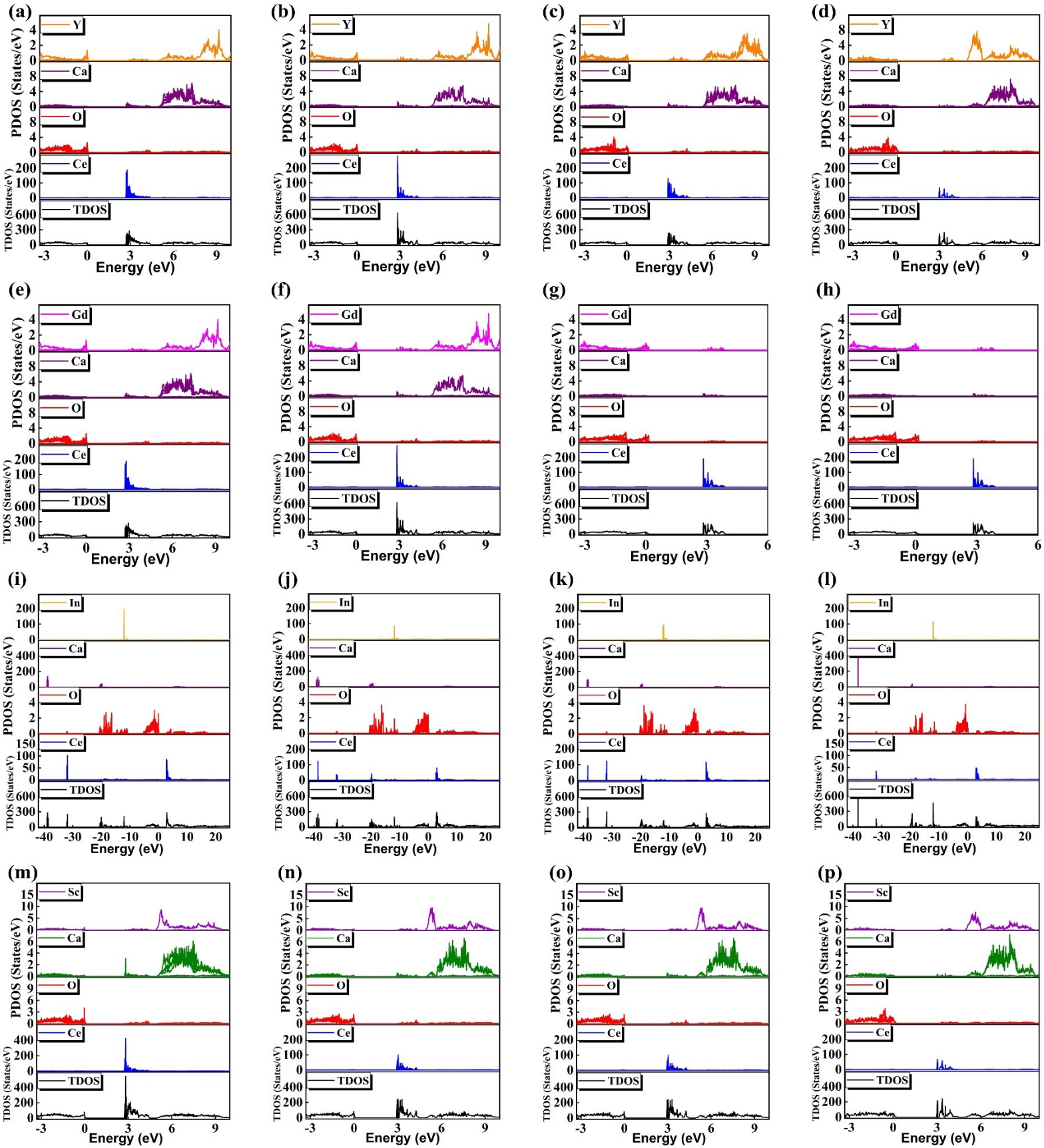

Fig S8: DFT simulated density of states of $CaCe_{1-x}M_xO_{3-\delta}$ (M = Y^{3+}, Gd^{3+}, In^{3+}, Sc^{3+}) corresponding to distinct doping concentration (x = 0.125, 0.25, 0.375, 0.5)

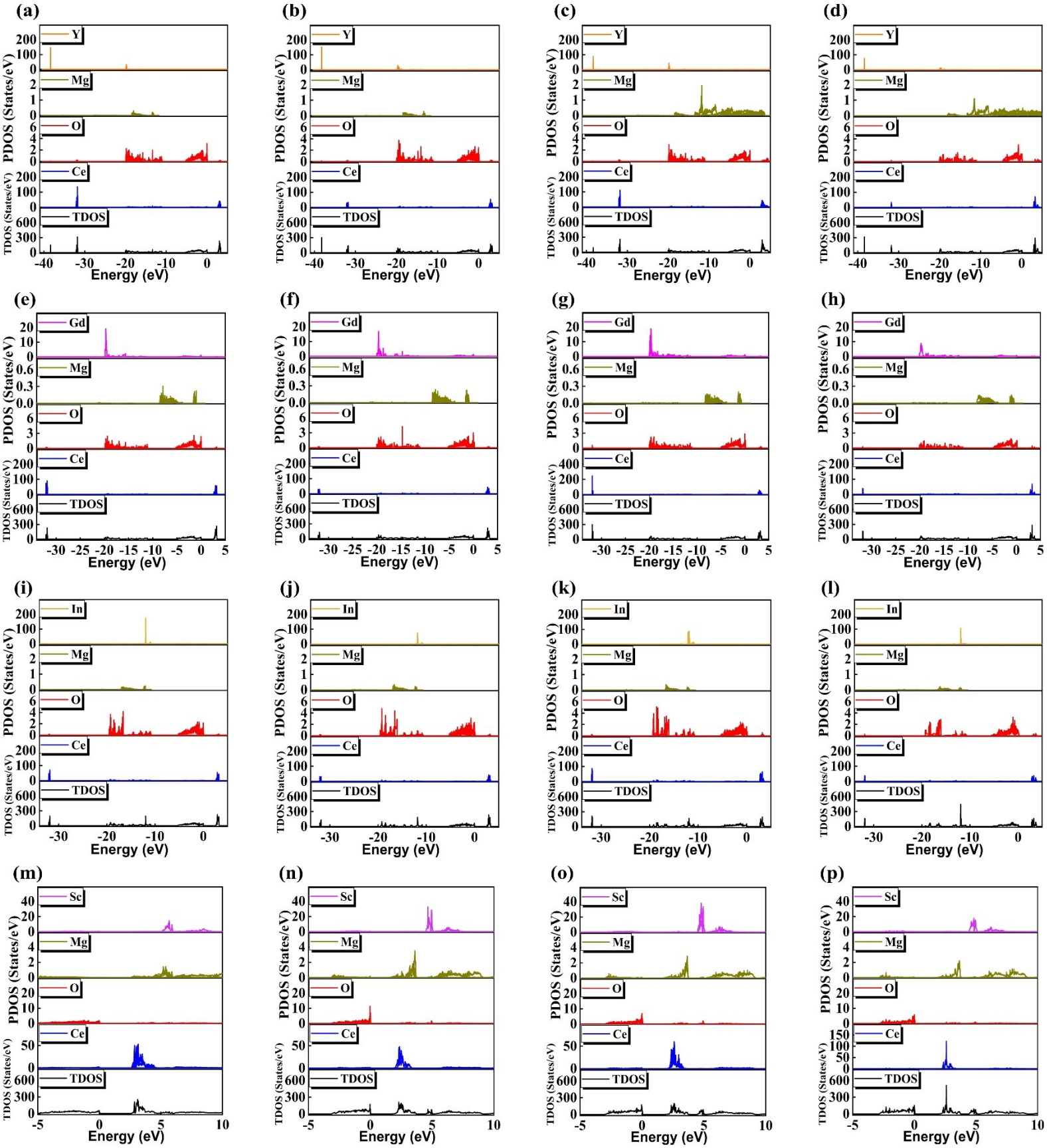

Fig S9: DFT simulated density of states of $MgCe_{1-x}M_xO_{3-\delta}$ (M = Y^{3+}, Gd^{3+}, In^{3+}, Sc^{3+}) corresponding to distinct doping concentration (x = 0.125, 0.25, 0.375, 0.5)

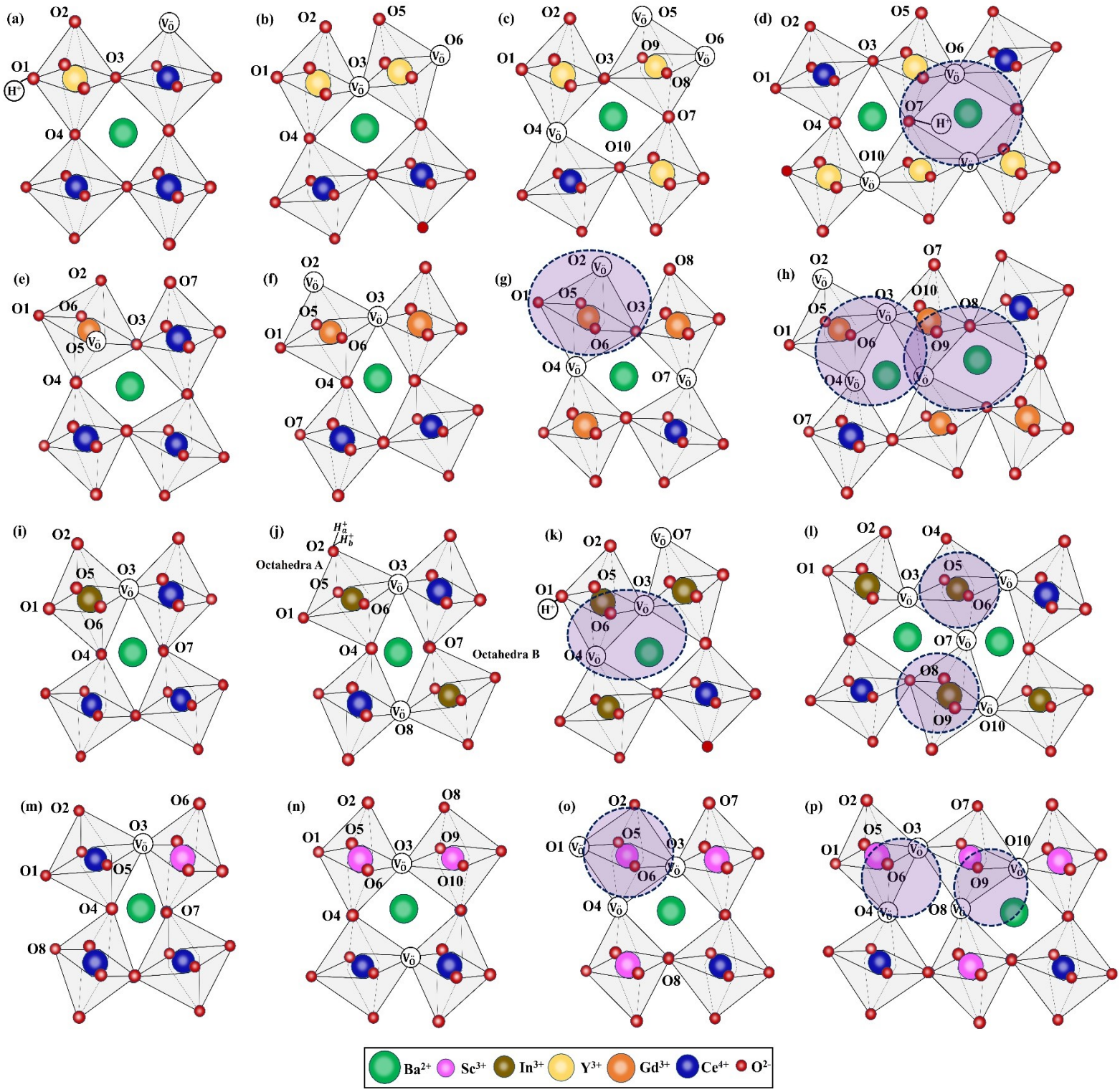

Fig S10: Proton landscape as function of different sized acceptors (M = Y^{3+}, Gd^{3+}, Sc^{3+}, In^{3+}) and doping concentration (x = 0.125, 0.25, 0.375, 0.5) in $BaCeO_3$

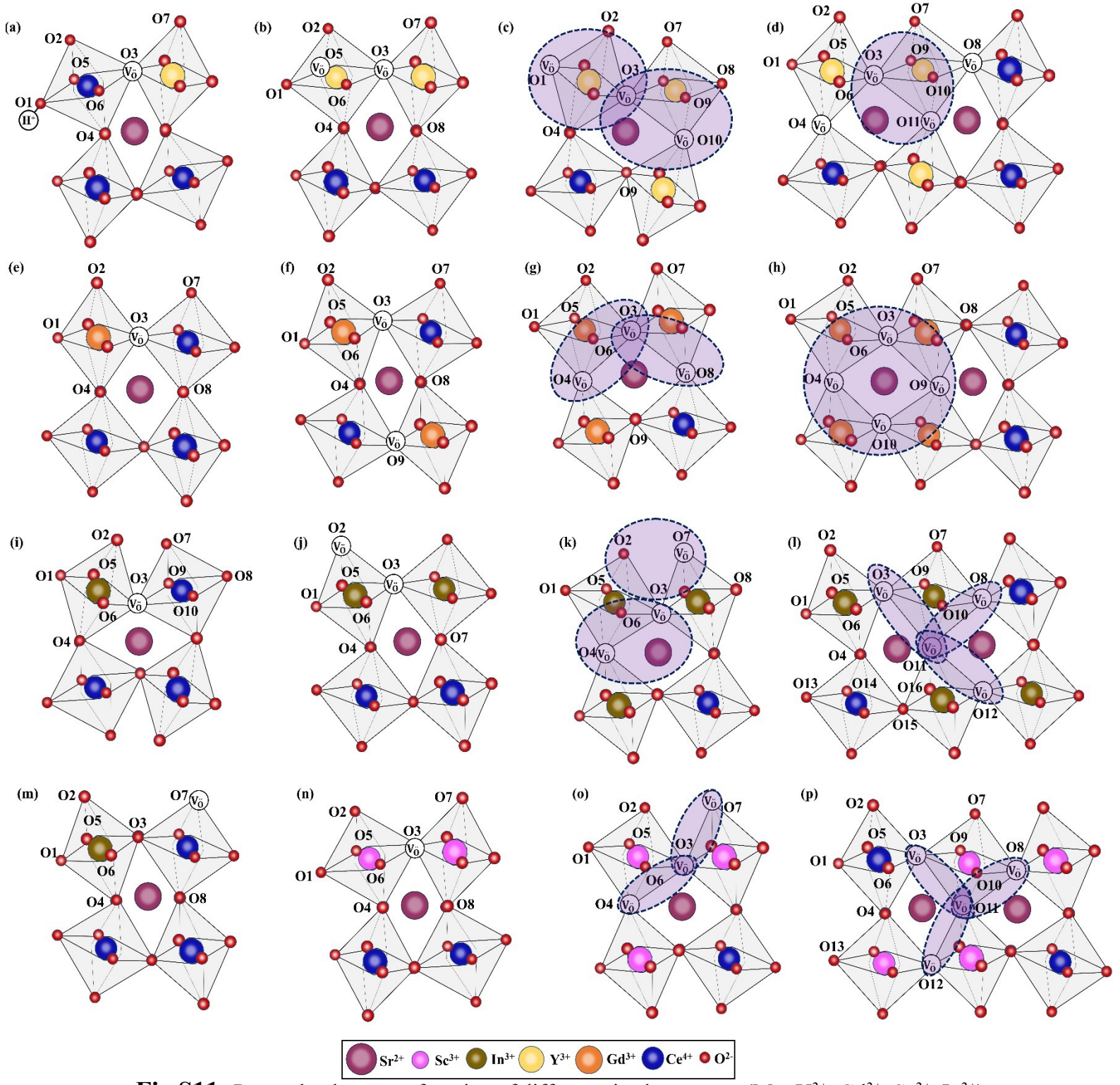

Fig S11: Proton landscape as function of different sized acceptors (M = Y^{3+}, Gd^{3+}, Sc^{3+}, In^{3+}) and doping concentration (x = 0.125, 0.25, 0.375, 0.5) in $SrCeO_3$

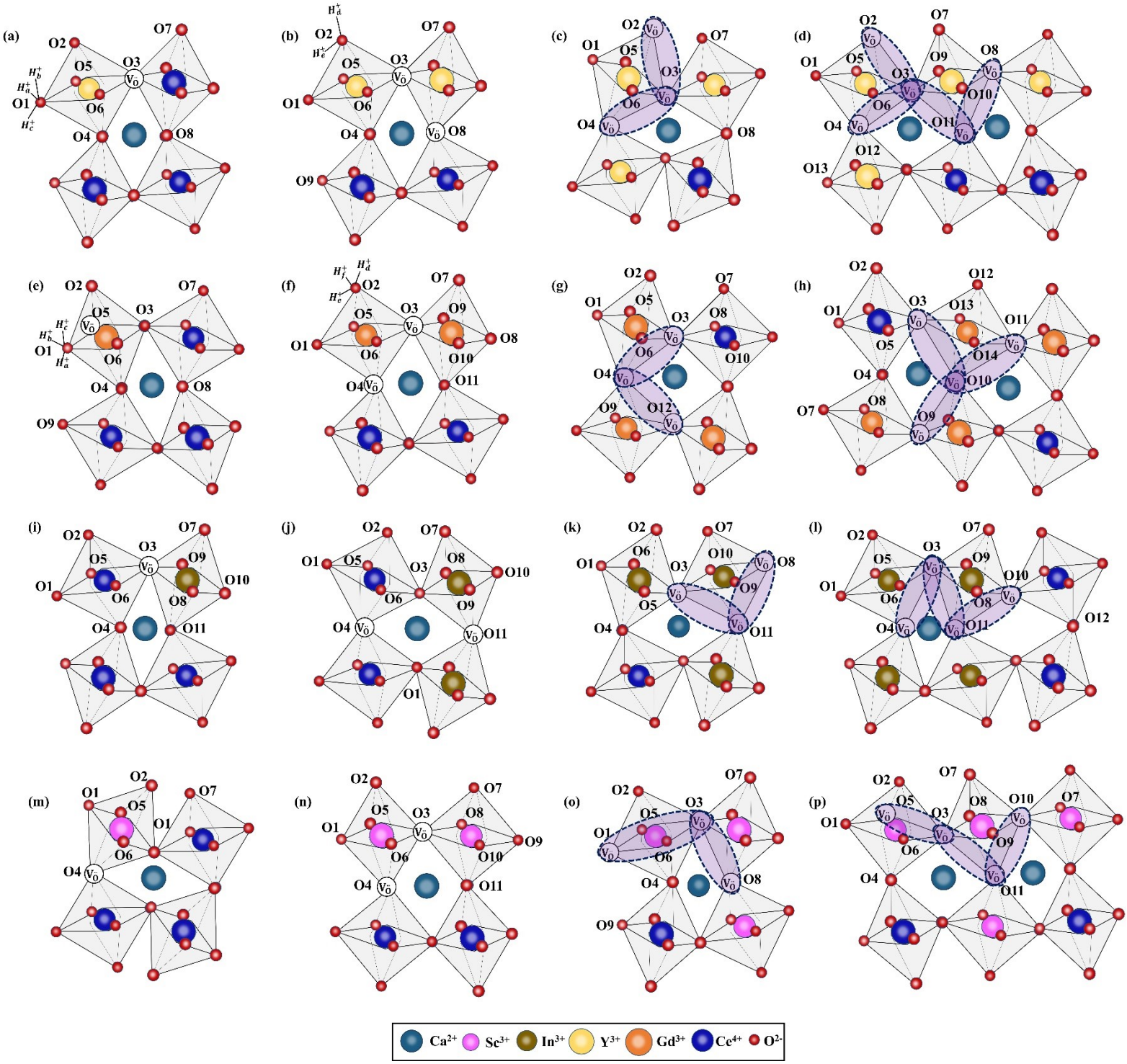

Fig S12: Proton landscape as function of different sized acceptors (M = Y^{3+}, Gd^{3+}, Sc^{3+}, In^{3+}) and doping concentration (x = 0.125, 0.25, 0.375, 0.5) in $CaCeO_3$

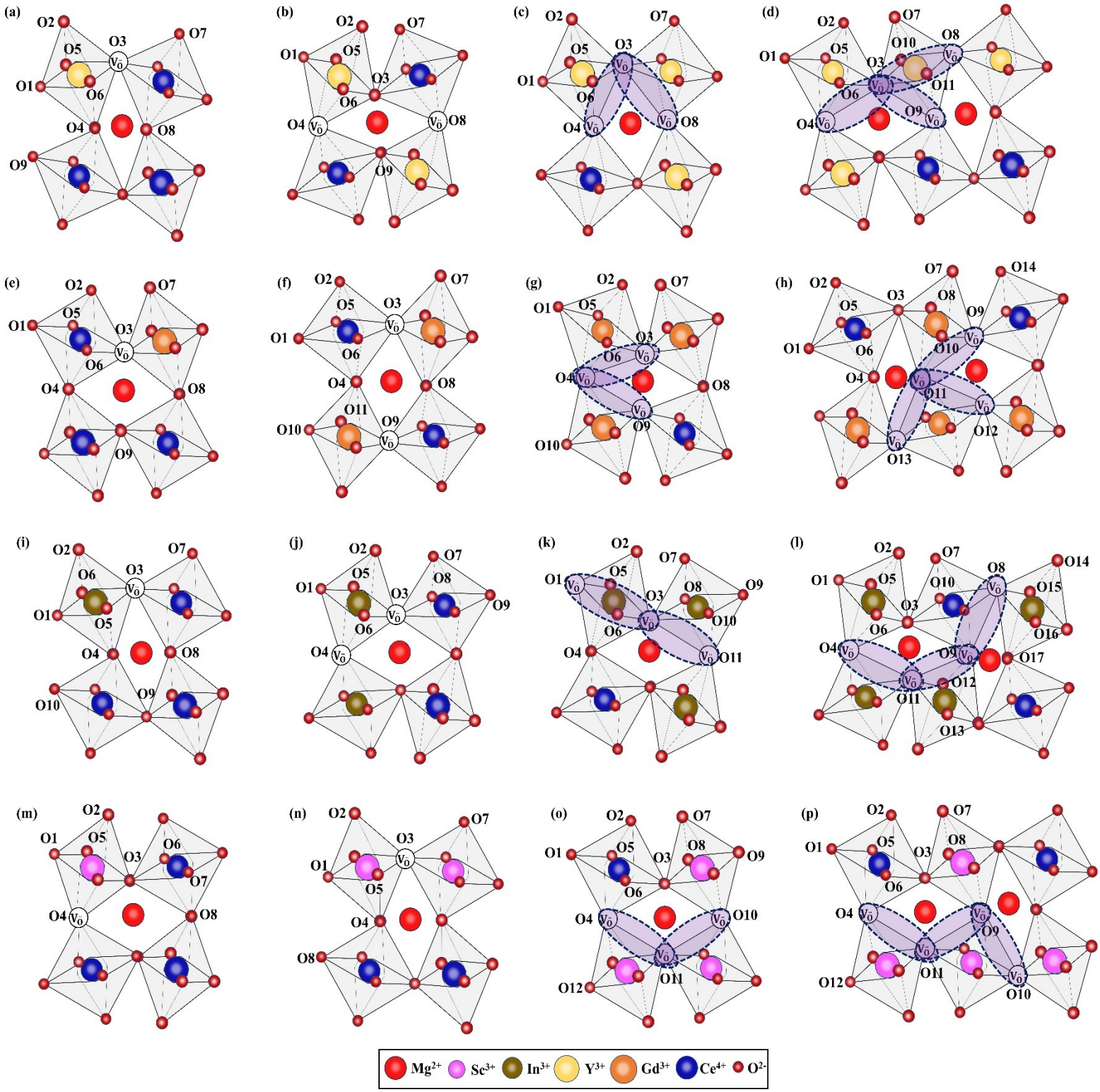

Fig S13: Proton landscape as function of different sized acceptors (M = Y^{3+}, Gd^{3+}, Sc^{3+}, In^{3+}) and doping concentration (x = 0.125, 0.25, 0.375, 0.5) in $MgCeO_3$

POTCAR file for Cerium (Ce):

PAW_PBE Ce 23Dec2003

12.0000000000000

parameters from PSCTR are:

VRHFIN =Ce : [core= Kr 4d10]

LEXCH = PE

EATOM = 1063.0861 eV, 78.1346 Ry

TITEL = PAW_PBE Ce 23Dec2003

LULTRA = F use ultrasoft PP ?

IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no

RPACOR = 1.800 partial core radius

POMASS = 140.115; ZVAL = 12.000 mass and valenz

RCORE = 2.700 outmost cutoff radius

RWIGS = 2.500; RWIGS = 1.323 wigner-seitz radius (au A)

ENMAX = 273.042; ENMIN = 204.781 eV

RCLOC = 1.810 cutoff for local pot

LCOR = T correct aug charges

LPAW = T paw PP

EAUG = 580.196

DEXC = 0.000

RMAX = 2.749 core radius for proj-oper

RAUG = 1.300 factor for augmentation sphere

RDEP = 2.810 radius for radial grids

RDEPT = 2.162 core radius for aug-charge

Atomic configuration

14 entries

n	l	j	E	occ.
1	0	0.50	-40258.9816	2.0000
2	0	0.50	-6445.4884	2.0000

2 1 1.50 -5771.7470 6.0000

3 0 0.50 -1387.9739 2.0000

3 1 1.50 -1173.8158 6.0000

3 2 2.50 -869.9108 10.0000

4 0 0.50 -280.8706 2.0000

4 1 1.50 -210.9815 6.0000

4 2 2.50 -110.4558 10.0000

5 0 0.50 -40.5819 2.0000

6 0 0.50 -3.7444 2.0000

5 1 1.50 -23.2188 6.0000

5 2 2.50 -3.0598 1.0000

4 3 2.50 -5.3970 1.0000

Description

l E TYP RCUT TYP RCUT

0 -40.5819164 23 1.500

0 -3.7443793 23 2.300

1 -23.2188445 23 2.000

1 40.8174780 23 2.300

2 -3.0597556 23 2.500

2 13.6058260 23 2.500

3 -5.3970469 23 2.700

3 -5.8505052 23 2.700

Error from kinetic energy argument (eV)

NDATA = 100

STEP = 20.000 1.050

227. 219. 215. 207. 202. 194. 185. 181.

172. 163. 159. 151. 142. 134. 126. 118.

111. 104. 96.6 86.7 80.5 74.6 66.4 61.3

56.5 49.9 43.9 40.2 35.2 30.7 26.7 23.2

20.1 17.3 14.9 12.8 10.4 8.89 7.15 6.06

4.82 3.81 2.99 2.33 1.79 1.37 1.03 0.713

0.525 0.355 0.238 0.175 0.123 0.928E-01 0.744E-01 0.680E-01

0.655E-01 0.643E-01 0.626E-01 0.593E-01 0.543E-01 0.478E-01 0.407E-01 0.324E-01

0.260E-01 0.199E-01 0.155E-01 0.128E-01 0.112E-01 0.108E-01 0.107E-01 0.105E-01

0.100E-01 0.910E-02 0.768E-02 0.632E-02 0.493E-02 0.389E-02 0.322E-02 0.297E-02

0.290E-02 0.286E-02 0.271E-02 0.240E-02 0.200E-02 0.161E-02 0.132E-02 0.113E-02

0.103E-02 0.983E-03 0.922E-03 0.841E-03 0.722E-03 0.606E-03 0.499E-03 0.427E-03

0.391E-03 0.377E-03 0.353E-03 0.307E-03

END of PSCTR-controll parameters

local part

POTCAR file for Scandium (Sc):

PAW_PBE Sc_sv 07Sep2000

11.0000000000000

parameters from PSCTR are:

VRHFIN =Sc: 3p4s3d

LEXCH = PE

EATOM = 1273.2868 eV, 93.5839 Ry

TITEL = PAW_PBE Sc_sv 07Sep2000

LULTRA = F use ultrasoft PP ?

IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no

RPACOR = 2.200 partial core radius

POMASS = 44.956; ZVAL = 11.000 mass and valenz

RCORE = 2.500 outmost cutoff radius

RWIGS = 2.700; RWIGS = 1.429 wigner-seitz radius (au A)

ENMAX = 222.660; ENMIN = 166.995 eV

RCLOC = 1.805 cutoff for local pot

LCOR = T correct aug charges

LPAW = T paw PP

EAUG = 443.063

RMAX = 2.551 core radius for proj-oper

RAUG = 1.300 factor for augmentation sphere

RDEP = 2.650 radius for radial grids

RDEPT = 2.038 core radius for aug-charge

Atomic configuration

8 entries

n	l	j	E	occ.
1	0	0.50	-4394.2533	2.0000
2	0	0.50	-471.0040	2.0000
2	1	1.50	-384.9788	6.0000
3	0	0.50	-52.1410	2.0000
4	0	0.50	-3.5584	1.0000
3	1	1.50	-30.8841	6.0000
3	2	2.50	-1.3655	2.0000
4	3	2.50	-1.3606	0.0000

Description

l	E	TYP	RCUT	TYP	RCUT
0	-52.1409870	23	1.800		
0	-3.5583698	23	2.500		
1	-30.8840697	23	2.300		
1	4.0817478	23	2.300		
2	-1.3655397	23	2.500		
2	0.3564476	23	2.500		

Error from kinetic energy argument (eV)

NDATA = 100

STEP = 20.000 1.050

177.	173.	170.	166.	164.	159.	154.	152.
146.	141.	139.	133.	128.	122.	116.	111.
105.	99.6	94.1	86.1	80.8	75.7	68.3	63.6
59.0	52.5	46.5	42.7	37.4	32.5	28.1	24.1
20.5	17.3	14.5	12.1	9.34	7.62	5.72	4.56

3.32 2.37 1.65 1.13 0.755 0.495 0.320 0.186

0.124 0.812E-01 0.614E-01 0.539E-01 0.488E-01 0.450E-01 0.398E-01 0.346E-01

0.290E-01 0.226E-01 0.171E-01 0.128E-01 0.983E-02 0.782E-02 0.649E-02 0.539E-02

0.462E-02 0.380E-02 0.304E-02 0.240E-02 0.186E-02 0.157E-02 0.138E-02 0.126E-02

0.113E-02 0.969E-03 0.751E-03 0.567E-03 0.412E-03 0.331E-03 0.305E-03 0.301E-03

0.285E-03 0.243E-03 0.188E-03 0.136E-03 0.107E-03 0.969E-04 0.926E-04 0.838E-04

0.699E-04 0.565E-04 0.464E-04 0.403E-04 0.343E-04 0.293E-04 0.257E-04 0.233E-04

0.200E-04 0.161E-04 0.128E-04 0.118E-04

END of PSCTR-controll parameters

local part

POTCAR file for Indium (In):

PAW_PBE In_d 06Sep2000

13.0000000000000

parameters from PSCTR are:

VRHFIN =In: s2p1

LEXCH = PE

EATOM = 1576.8302 eV, 115.8937 Ry

TITEL = PAW_PBE In_d 06Sep2000

LULTRA = F use ultrasoft PP ?

IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no

RPACOR = 2.200 partial core radius

POMASS = 114.820; ZVAL = 13.000 mass and valenz

RCORE = 2.500 outmost cutoff radius

RWIGS = 3.170; RWIGS = 1.677 wigner-seitz radius (au A)

ENMAX = 239.211; ENMIN = 179.409 eV

ICORE = 3 local potential

LCOR = T correct aug charges

LPAW = T paw PP

EAUG = 449.704

DEXC = 0.000

RMAX = 2.552 core radius for proj-oper

RAUG = 1.300 factor for augmentation sphere

RDEP = 2.630 radius for radial grids

RDEPT = 2.033 core radius for aug-charge

Atomic configuration

12 entries

n	l	j	E	occ.
1	0	0.50	-27747.9169	2.0000
2	0	0.50	-4154.4438	2.0000
2	1	1.50	-3728.4305	6.0000
3	0	0.50	-788.3680	2.0000
3	1	1.50	-648.9215	6.0000
3	2	2.50	-432.5893	10.0000
4	0	0.50	-119.6363	2.0000
4	1	1.50	-78.1086	6.0000
4	2	2.50	-18.6227	10.0000
5	0	0.50	-8.2107	2.0000
5	1	0.50	-2.5185	1.0000
4	3	2.50	-2.7212	0.0000

Description

l	E	TYP	RCUT	TYP	RCUT
2	-18.6226981	23	2.500		
2	-1.3605826	23	2.500		
0	-8.2107305	23	2.500		
0	-6.1485975	23	2.500		
1	-2.5184867	23	2.500		
1	3.2427302	23	2.500		
3	-1.3605826	7	2.500		

Error from kinetic energy argument (eV)

NDATA = 100

STEP = 20.000 1.050

128. 127. 126. 125. 124. 122. 120. 119.

117. 115. 114. 111. 109. 106. 103. 99.8

96.7 93.4 90.0 84.8 81.3 77.7 72.2 68.6

65.0 59.6 54.3 50.9 45.9 41.1 36.5 32.3

28.3 24.6 21.2 18.1 14.5 12.2 9.46 7.73

5.81 4.27 3.06 2.14 1.45 0.955 0.607 0.329

0.197 0.105 0.642E-01 0.514E-01 0.471E-01 0.468E-01 0.450E-01 0.408E-01

0.346E-01 0.259E-01 0.179E-01 0.117E-01 0.768E-02 0.561E-02 0.485E-02 0.471E-02

0.463E-02 0.425E-02 0.353E-02 0.266E-02 0.179E-02 0.128E-02 0.100E-02 0.937E-03

0.921E-03 0.852E-03 0.691E-03 0.521E-03 0.368E-03 0.288E-03 0.266E-03 0.259E-03

0.232E-03 0.182E-03 0.133E-03 0.103E-03 0.947E-04 0.911E-04 0.791E-04 0.594E-04

0.449E-04 0.400E-04 0.383E-04 0.335E-04 0.250E-04 0.200E-04 0.185E-04 0.172E-04

0.136E-04 0.107E-04 0.961E-05 0.895E-05

END of PSCTR-controll parameters

local part

POTCAR file for Yttrium (Y):

PAW_PBE Y_sv 25May2007

11.0000000000000

parameters from PSCTR are:

VRHFIN =Y: 4s4p5s4d

LEXCH = PE

EATOM = 1046.9140 eV, 76.9460 Ry

TITEL = PAW_PBE Y_sv 25May2007

LULTRA = F use ultrasoft PP ?

IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no

RPACOR = 2.200 partial core radius

POMASS = 88.906; ZVAL = 11.000 mass and valenz

RCORE = 2.800 outmost cutoff radius

RWIGS = 3.430; RWIGS = 1.815 wigner-seitz radius (au A)

ENMAX = 202.626; ENMIN = 151.970 eV

RCLOC = 2.212 cutoff for local pot

LCOR = T correct aug charges

LPAW = T paw PP

EAUG = 470.889

DEXC = 0.000

RMAX = 2.863 core radius for proj-oper

RAUG = 1.300 factor for augmentation sphere

RDEP = 2.926 radius for radial grids

RDEPT = 2.280 core radius for aug-charge

Atomic configuration

11 entries

n	l	j	E	occ.
1	0	0.50	-16863.0720	2.0000
2	0	0.50	-2309.2881	2.0000
2	1	1.50	-2055.5536	6.0000
3	0	0.50	-367.1837	2.0000
3	1	1.50	-284.8912	6.0000
3	2	2.50	-149.4324	10.0000
4	0	0.50	-46.3345	2.0000
5	0	0.50	-3.6387	1.0000
4	1	1.50	-26.3769	6.0000
4	2	2.50	-1.6291	2.0000
4	3	2.50	-1.3606	0.0000

Description

l	E	TYP	RCUT	TYP	RCUT
0	-46.3344714	23	2.600		
0	-3.6387002	23	2.700		

1 -26.3769044 23 2.600

1 -27.7374870 23 2.600

2 -1.6291019 23 2.600

2 0.1354037 23 2.600

3 -1.3605826 23 2.800

Error from kinetic energy argument (eV)

NDATA = 100

STEP = 20.000 1.050

159. 154. 151. 145. 142. 136. 130. 127.

121. 115. 111. 105. 99.0 92.8 86.8 81.0

75.3 69.7 64.4 56.9 52.1 47.6 41.3 37.4

33.8 28.8 24.3 21.6 18.0 14.9 12.2 9.90

7.96 6.33 4.98 3.88 2.73 2.07 1.40 1.03

0.677 0.436 0.279 0.180 0.119 0.832E-01 0.626E-01 0.484E-01

0.415E-01 0.351E-01 0.294E-01 0.251E-01 0.200E-01 0.155E-01 0.112E-01 0.858E-02

0.674E-02 0.533E-02 0.446E-02 0.385E-02 0.334E-02 0.283E-02 0.234E-02 0.182E-02

0.146E-02 0.115E-02 0.951E-03 0.822E-03 0.710E-03 0.618E-03 0.510E-03 0.410E-03

0.329E-03 0.272E-03 0.232E-03 0.207E-03 0.179E-03 0.149E-03 0.119E-03 0.989E-04

0.844E-04 0.747E-04 0.652E-04 0.539E-04 0.438E-04 0.370E-04 0.327E-04 0.287E-04

0.240E-04 0.198E-04 0.168E-04 0.151E-04 0.129E-04 0.108E-04 0.904E-05 0.804E-05

0.701E-05 0.589E-05 0.494E-05 0.444E-05

END of PSCTR-controll parameters

local part

POTCAR file for Gadolinium (Gd):

PAW_PBE Gd_3 06Sep2000

9.00000000000000

parameters from PSCTR are:

VRHFIN =Gd : [core=Xe4]

LEXCH = PE

EATOM = 630.6592 eV, 46.3521 Ry

TITEL = PAW_PBE Gd_3 06Sep2000

LULTRA = F use ultrasoft PP ?

IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no

RPACOR = 2.300 partial core radius

POMASS = 157.250; ZVAL = 9.000 mass and valenz

RCORE = 3.000 outmost cutoff radius

RWIGS = 3.000; RWIGS = 1.588 wigner-seitz radius (au A)

ENMAX = 154.332; ENMIN = 115.749 eV

RCLOC = 2.316 cutoff for local pot

LCOR = T correct aug charges

LPAW = T paw PP

EAUG = 282.292

DEXC = 0.000

RMAX = 3.070 core radius for proj-oper

RAUG = 1.300 factor for augmentation sphere

RDEP = 3.114 radius for radial grids

RDEPT = 2.525 core radius for aug-charge

Atomic configuration

14 entries

n	l	j	E	occ.
1	0	0.50	-50087.2354	2.0000
2	0	0.50	-8269.2182	2.0000
2	1	1.50	-7357.3672	6.0000
3	0	0.50	-1833.2681	2.0000
3	1	1.50	-1550.9376	6.0000
3	2	2.50	-1178.7203	10.0000
4	0	0.50	-369.2977	2.0000
4	1	1.50	-276.2600	6.0000
4	2	2.50	-147.6610	10.0000

4 3 2.50 -8.7140 7.0000

5 0 0.50 -49.7259 2.0000

6 0 0.50 -4.1254 2.0000

5 1 1.50 -27.2537 6.0000

5 2 2.50 -2.5337 1.0000

Description

l E TYP RCUT TYP RCUT

0 -4.1254075 23 3.000

0 6.8029130 23 3.000

1 -27.2537268 23 3.000

1 -28.6143094 23 3.000

2 -2.5337233 23 3.000

2 0.2512192 23 3.000

Error from kinetic energy argument (eV)

NDATA = 100

STEP = 20.000 1.050

67.1 64.1 62.5 59.3 57.7 54.4 51.1 49.4

46.1 42.8 41.2 38.0 34.9 31.9 29.0 26.2

23.6 21.2 18.9 15.8 13.9 12.1 9.83 8.47

7.26 5.69 4.39 3.67 2.75 2.03 1.47 1.05

0.730 0.499 0.336 0.223 0.130 0.887E-01 0.577E-01 0.454E-01

0.366E-01 0.317E-01 0.279E-01 0.240E-01 0.200E-01 0.159E-01 0.122E-01 0.844E-02

0.628E-02 0.455E-02 0.364E-02 0.326E-02 0.297E-02 0.271E-02 0.230E-02 0.190E-02

0.150E-02 0.109E-02 0.807E-03 0.655E-03 0.585E-03 0.545E-03 0.496E-03 0.413E-03

0.332E-03 0.248E-03 0.193E-03 0.166E-03 0.152E-03 0.141E-03 0.119E-03 0.926E-04

0.711E-04 0.592E-04 0.541E-04 0.505E-04 0.432E-04 0.339E-04 0.262E-04 0.232E-04

0.218E-04 0.192E-04 0.153E-04 0.120E-04 0.108E-04 0.101E-04 0.857E-05 0.667E-05

0.570E-05 0.537E-05 0.462E-05 0.370E-05 0.316E-05 0.298E-05 0.251E-05 0.201E-05

0.184E-05 0.167E-05 0.132E-05 0.117E-05

END of PSCTR-controll parameters

local part

POTCAR file for Oxygen (O):

PAW_PBE O 08Apr2002

6.00000000000000

parameters from PSCTR are:

VRHFIN =O: s2p4

LEXCH = PE

EATOM = 432.3788 eV, 31.7789 Ry

TITEL = PAW_PBE O 08Apr2002

LULTRA = F use ultrasoft PP ?

IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no

RPACOR = 1.200 partial core radius

POMASS = 16.000; ZVAL = 6.000 mass and valenz

RCORE = 1.520 outmost cutoff radius

RWIGS = 1.550; RWIGS = 0.820 wigner-seitz radius (au A)

ENMAX = 400.000; ENMIN = 300.000 eV

ICORE = 2 local potential

LCOR = T correct aug charges

LPAW = T paw PP

EAUG = 605.392

DEXC = 0.000

RMAX = 1.553 core radius for proj-oper

RAUG = 1.300 factor for augmentation sphere

RDEP = 1.550 radius for radial grids

RDEPT = 1.329 core radius for aug-charge

Atomic configuration

4 entries

n l j E occ.

1 0 0.50 -514.6923 2.0000

2 0 0.50 -23.9615 2.0000

2 1 0.50 -9.0305 4.0000

3 2 1.50 -9.5241 0.0000

Description

l E TYP RCUT TYP RCUT

0 -23.9615318 23 1.200

0 -9.5240782 23 1.200

1 -9.0304911 23 1.520

1 8.1634956 23 1.520

2 -9.5240782 7 1.500

Error from kinetic energy argument (eV)

NDATA = 100

STEP = 20.000 1.050

163. 160. 159. 156. 154. 151. 148. 146.

142. 139. 137. 134. 130. 126. 123. 119.

115. 111. 108. 102. 98.8 95.2 90.0 86.6

83.2 78.3 73.5 70.4 65.9 61.6 57.4 53.4

49.6 46.0 42.6 39.3 35.3 32.4 28.9 26.4

23.4 20.6 18.1 15.8 13.7 11.9 10.3 8.47

7.22 5.87 4.73 3.95 3.13 2.45 1.80 1.37

1.03 0.721 0.493 0.329 0.215 0.138 0.882E-01 0.534E-01

0.367E-01 0.267E-01 0.223E-01 0.205E-01 0.193E-01 0.181E-01 0.162E-01 0.138E-01

0.112E-01 0.878E-02 0.646E-02 0.490E-02 0.370E-02 0.300E-02 0.259E-02 0.238E-02

0.219E-02 0.196E-02 0.167E-02 0.132E-02 0.100E-02 0.764E-03 0.617E-03 0.544E-03

0.522E-03 0.507E-03 0.467E-03 0.403E-03 0.312E-03 0.236E-03 0.181E-03 0.157E-03

0.152E-03 0.150E-03 0.139E-03 0.118E-03

END of PSCTR-controll parameters

local part

POTCAR file for Barium (Ba):

PAW_PBE Ba_sv 06Sep2000

10.0000000000000

parameters from PSCTR are:

VRHFIN =Ba: 5s5p6s

LEXCH = PE

EATOM = 700.8560 eV, 51.5115 Ry

TITEL = PAW_PBE Ba_sv 06Sep2000

LULTRA = F use ultrasoft PP ?

IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no

RPACOR = 2.400 partial core radius

POMASS = 137.327; ZVAL = 10.000 mass and valenz

RCORE = 2.800 outmost cutoff radius

RWIGS = 3.740; RWIGS = 1.979 wigner-seitz radius (au A)

ENMAX = 187.181; ENMIN = 140.386 eV

RCLOC = 2.516 cutoff for local pot

LCOR = T correct aug charges

LPAW = T paw PP

EAUG = 351.165

DEXC = 0.000

RMAX = 2.865 core radius for proj-oper

RAUG = 1.300 factor for augmentation sphere

RDEP = 2.976 radius for radial grids

RDEPT = 2.289 core radius for aug-charge

Atomic configuration

13 entries

n	l	j	E	occ.
1	0	0.50	-37249.5946	2.0000
2	0	0.50	-5887.1925	2.0000
2	1	1.50	-5278.3977	6.0000
3	0	0.50	-1242.7293	2.0000

3 1 1.50 -1047.6609 6.0000

3 2 2.50 -764.6158 10.0000

4 0 0.50 -243.8228 2.0000

4 1 1.50 -180.9218 6.0000

4 2 2.50 -89.6477 10.0000

5 0 0.50 -33.6549 2.0000

6 0 0.50 -3.2247 1.9900

5 1 1.50 -18.7193 6.0000

5 2 2.50 -2.0115 0.0100

Description

l E TYP RCUT TYP RCUT

0 -33.6549039 23 2.800

0 -3.2246942 23 2.800

1 -18.7193050 23 2.700

1 27.2116520 23 2.700

2 -2.0115002 23 2.700

2 0.3057420 23 2.700

Error from kinetic energy argument (eV)

NDATA = 100

STEP = 20.000 1.050

143. 135. 132. 124. 120. 113. 106. 102.

94.9 87.9 84.5 77.9 71.6 65.5 59.7 54.3

49.1 44.3 39.8 33.7 30.0 26.6 22.1 19.4

16.9 13.7 11.0 9.50 7.50 5.86 4.53 3.46

2.61 1.94 1.42 1.03 0.650 0.454 0.275 0.187

0.112 0.695E-01 0.472E-01 0.363E-01 0.312E-01 0.285E-01 0.265E-01 0.236E-01

0.208E-01 0.169E-01 0.131E-01 0.103E-01 0.741E-02 0.533E-02 0.379E-02 0.312E-02

0.280E-02 0.262E-02 0.246E-02 0.221E-02 0.188E-02 0.150E-02 0.114E-02 0.829E-03

0.665E-03 0.574E-03 0.544E-03 0.520E-03 0.465E-03 0.389E-03 0.295E-03 0.221E-03

0.182E-03 0.168E-03 0.163E-03 0.152E-03 0.126E-03 0.970E-04 0.747E-04 0.672E-04

0.656E-04 0.615E-04 0.515E-04 0.393E-04 0.324E-04 0.311E-04 0.301E-04 0.255E-04

0.198E-04 0.168E-04 0.164E-04 0.154E-04 0.122E-04 0.985E-05 0.939E-05 0.892E-05

0.715E-05 0.588E-05 0.568E-05 0.521E-05

END of PSCTR-controll parameters

local part

POTCAR file for Strontium (Sr):

PAW_PBE Sr_sv 07Sep2000

10.0000000000000

parameters from PSCTR are:

VRHFIN =Sr: 4s4p5s

LEXCH = PE

EATOM = 843.0319 eV, 61.9611 Ry

TITEL = PAW_PBE Sr_sv 07Sep2000

LULTRA = F use ultrasoft PP ?

IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no

RPACOR = 2.200 partial core radius

POMASS = 87.620; ZVAL = 10.000 mass and valenz

RCORE = 2.500 outmost cutoff radius

RWIGS = 4.040; RWIGS = 2.138 wigner-seitz radius (au A)

ENMAX = 229.353; ENMIN = 172.014 eV

RCLOC = 2.201 cutoff for local pot

LCOR = T correct aug charges

LPAW = T paw PP

EAUG = 366.804

DEXC = 0.000

RMAX = 2.547 core radius for proj-oper

RAUG = 1.300 factor for augmentation sphere

RDEP = 2.562 radius for radial grids

RDEPT = 2.128 core radius for aug-charge

Atomic configuration

10 entries

n	l	j	E	occ.
1	0	0.50	-15934.8930	2.0000
2	0	0.50	-2157.6250	2.0000
2	1	1.50	-1917.0034	6.0000
3	0	0.50	-333.7288	2.0000
3	1	1.50	-256.0992	6.0000
3	2	2.50	-127.9971	10.0000
4	0	0.50	-40.8953	2.0000
5	0	0.50	-3.5257	1.9990
4	1	1.50	-22.8179	6.0000
4	2	1.50	-1.2815	0.0010

Description

l	E	TYP	RCUT	TYP	RCUT
0	-40.8953213	23	2.480		
0	-3.5257161	23	2.480		
1	-22.8178632	23	2.500		
1	-24.1784458	23	2.500		
2	-1.2814598	23	2.500		
2	0.2279365	23	2.500		

Error from kinetic energy argument (eV)

NDATA = 100

STEP = 20.000 1.050

168. 163. 160. 153. 150. 144. 137. 134.

127. 121. 117. 111. 104. 97.6 91.3 85.2

79.2 73.5 68.0 60.1 55.1 50.5 43.9 39.9

36.1 30.9 26.3 23.5 19.7 16.4 13.6 11.1

9.07 7.31 5.85 4.63 3.35 2.59 1.82 1.38

0.942 0.634 0.422 0.281 0.189 0.130 0.928E-01 0.654E-01

0.523E-01 0.415E-01 0.338E-01 0.287E-01 0.232E-01 0.184E-01 0.137E-01 0.107E-01

0.841E-02 0.651E-02 0.528E-02 0.447E-02 0.387E-02 0.335E-02 0.285E-02 0.230E-02

0.187E-02 0.147E-02 0.118E-02 0.984E-03 0.839E-03 0.745E-03 0.643E-03 0.539E-03

0.438E-03 0.353E-03 0.285E-03 0.247E-03 0.217E-03 0.192E-03 0.160E-03 0.132E-03

0.106E-03 0.888E-04 0.786E-04 0.696E-04 0.591E-04 0.481E-04 0.395E-04 0.340E-04

0.306E-04 0.267E-04 0.218E-04 0.181E-04 0.158E-04 0.143E-04 0.122E-04 0.100E-04

0.856E-05 0.784E-05 0.678E-05 0.561E-05

END of PSCTR-controll parameters

local part

POTCAR file for Calcium (Ca):

PAW_PBE Ca_sv 06Sep2000

10.0000000000000

parameters from PSCTR are:

VRHFIN =Ca: 3s3p4s

LEXCH = PE

EATOM = 1006.0909 eV, 73.9456 Ry

TITEL = PAW_PBE Ca_sv 06Sep2000

LULTRA = F use ultrasoft PP ?

IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no

RPACOR = 2.000 partial core radius

POMASS = 40.078; ZVAL = 10.000 mass and valenz

RCORE = 2.300 outmost cutoff radius

RWIGS = 2.500; RWIGS = 1.323 wigner-seitz radius (au A)

ENMAX = 266.622; ENMIN = 199.967 eV

RCLOC = 1.808 cutoff for local pot

LCOR = T correct aug charges

LPAW = T paw PP

EAUG = 420.852

RMAX = 2.359 core radius for proj-oper

RAUG = 1.300 factor for augmentation sphere

RDEP = 2.392 radius for radial grids

RDEPT = 1.987 core radius for aug-charge

Atomic configuration

7 entries

n	l	j	E	occ.
1	0	0.50	-3949.1705	2.0000
2	0	0.50	-414.3434	2.0000
2	1	1.50	-334.7047	6.0000
3	0	0.50	-47.0896	2.0000
4	0	0.50	-3.7663	2.0000
3	1	1.50	-28.0061	6.0000
3	2	1.50	-4.0817	0.0000

Description

l	E	TYP	RCUT	TYP	RCUT
0	-47.0896403	23	2.300		
0	-3.7663320	23	2.300		
1	-28.0060855	23	2.300		
1	6.8029130	23	2.300		
2	-4.0817478	23	2.300		
2	0.4464412	23	2.300		

Error from kinetic energy argument (eV)

NDATA = 100

STEP = 20.000 1.050

175.	171.	169.	164.	162.	157.	152.	149.
144.	138.	136.	130.	124.	119.	113.	107.
102.	96.2	90.7	82.8	77.6	72.6	65.5	60.9
56.5	50.2	44.4	40.8	35.8	31.2	27.0	23.2
19.9	16.9	14.2	11.9	9.34	7.71	5.89	4.78
3.57	2.62	1.90	1.36	0.958	0.666	0.458	0.286

0.196 0.126 0.850E-01 0.651E-01 0.497E-01 0.401E-01 0.322E-01 0.269E-01
0.224E-01 0.175E-01 0.135E-01 0.103E-01 0.799E-02 0.633E-02 0.518E-02 0.426E-02
0.367E-02 0.310E-02 0.258E-02 0.212E-02 0.167E-02 0.136E-02 0.110E-02 0.916E-03
0.786E-03 0.680E-03 0.572E-03 0.483E-03 0.395E-03 0.325E-03 0.268E-03 0.232E-03
0.201E-03 0.172E-03 0.145E-03 0.118E-03 0.981E-04 0.839E-04 0.732E-04 0.625E-04
0.522E-04 0.433E-04 0.362E-04 0.316E-04 0.271E-04 0.229E-04 0.189E-04 0.160E-04
0.139E-04 0.120E-04 0.990E-05 0.835E-05
END of PSCTR-controll parameters
local part

POTCAR file for Magnesium (Mg):

PAW_PBE Mg 13Apr2007
2.00000000000000
parameters from PSCTR are:
VRHFIN =Mg: s2p0
LEXCH = PE
EATOM = 23.0369 eV, 1.6932 Ry

TITEL = PAW_PBE Mg 13Apr2007
LULTRA = F use ultrasoft PP ?
IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no
RPACOR = 1.500 partial core radius
POMASS = 24.305; ZVAL = 2.000 mass and valenz
RCORE = 2.000 outmost cutoff radius
RWIGS = 2.880; RWIGS = 1.524 wigner-seitz radius (au A)
ENMAX = 200.000; ENMIN = 100.000 eV
RCLOC = 1.506 cutoff for local pot
LCOR = T correct aug charges
LPAW = T paw PP
EAUG = 454.734

DEXC = 0.000

RMAX = 2.045 core radius for proj-oper

RAUG = 1.300 factor for augmentation sphere

RDEP = 2.025 radius for radial grids

RDEPT = 1.942 core radius for aug-charge

Atomic configuration

6 entries

n	l	j	E	occ.
1	0	0.50	-1259.6230	2.0000
2	0	0.50	-79.8442	2.0000
2	1	1.50	-46.6121	6.0000
3	0	0.50	-4.7055	2.0000
3	1	0.50	-1.3660	0.0000
3	2	1.50	-1.3606	0.0000

Description

l	E	TYP	RCUT	TYP	RCUT
0	-4.7054661	23	2.000		
0	27.2116520	23	2.000		
1	1.3605826	23	2.000		
1	27.2116520	23	2.000		
2	-1.3605826	23	2.000		

Error from kinetic energy argument (eV)

NDATA = 100

STEP = 20.000 1.050

1.04 1.04 1.04 1.03 1.02 1.01 0.987 0.975

0.946 0.913 0.895 0.855 0.813 0.768 0.721 0.674

0.626 0.579 0.532 0.465 0.423 0.382 0.326 0.291

0.259 0.215 0.177 0.154 0.125 0.994E-01 0.783E-01 0.609E-01

0.466E-01 0.352E-01 0.262E-01 0.192E-01 0.123E-01 0.874E-02 0.545E-02 0.385E-02

0.252E-02 0.183E-02 0.152E-02 0.142E-02 0.140E-02 0.140E-02 0.137E-02 0.128E-02

0.117E-02 0.990E-03 0.798E-03 0.649E-03 0.485E-03 0.355E-03 0.248E-03 0.195E-03

0.167E-03 0.155E-03 0.153E-03 0.152E-03 0.146E-03 0.133E-03 0.115E-03 0.911E-04

0.716E-04 0.533E-04 0.413E-04 0.353E-04 0.332E-04 0.331E-04 0.324E-04 0.299E-04

0.256E-04 0.206E-04 0.155E-04 0.124E-04 0.106E-04 0.102E-04 0.102E-04 0.970E-05

0.843E-05 0.674E-05 0.524E-05 0.428E-05 0.399E-05 0.398E-05 0.379E-05 0.325E-05

0.256E-05 0.204E-05 0.184E-05 0.182E-05 0.173E-05 0.148E-05 0.116E-05 0.976E-06

0.939E-06 0.920E-06 0.799E-06 0.641E-06

END of PSCTR-controll parameters

local part

VASP-POTCAR file comprising of frozen-core and valence electron configuration across different atomic components within standalone and acceptor (M = Sc^{3+}, In^{3+}, Y^{3+}, Gd^{3+}) doped $ACe_{1-x}M_xO_{3-\delta}$ (A = Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}) proton conductors