Supplementary Informations

Defect Properties and Solution Energies of Dopants in NASICON-Type $LiGe_2(PO_4)_3$ Solid Electrolyte: A First-Principles Study

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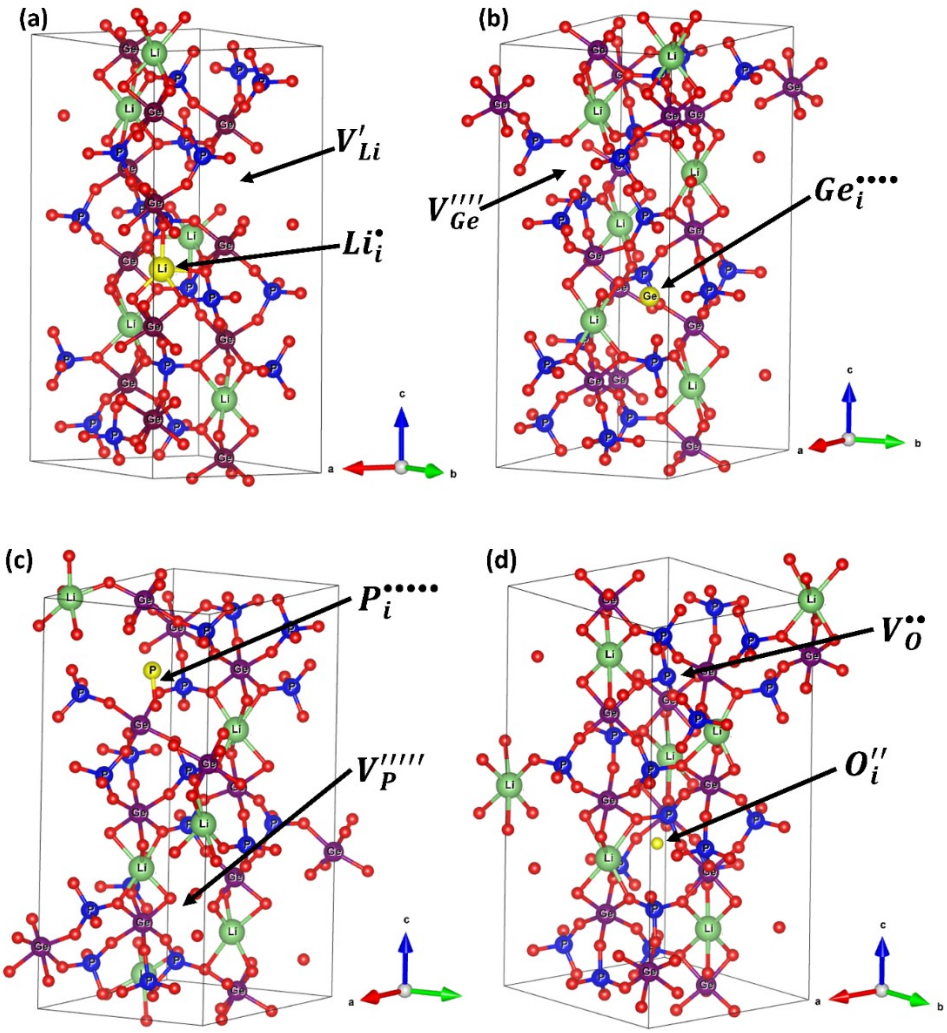


Fig. SI1: Optimized unit cell of LGP containing different kinds of Frenkel defects

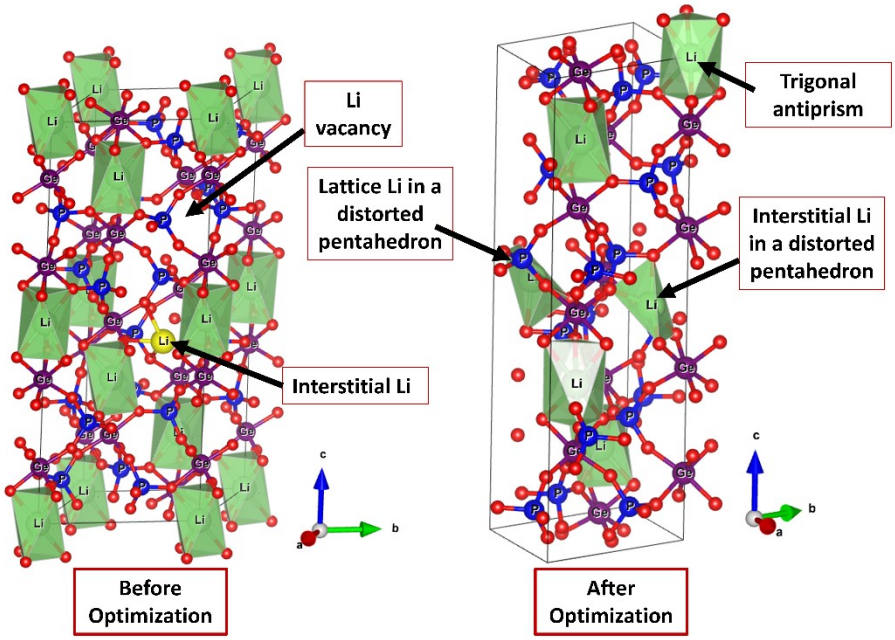


Fig. SI2: Close observation on the structure with Li Frenkel defect

Table SI1: Defects formation energies (eV/defect) reported previously			
Li–TM antisite defects (at 1000 K) Li–Ni antisite defect concentration Li–Co antisite defect concentration	 12.9% 0.002%	$Li_{12}TM_{12}O_{24}$ DFT calculations	[1]
Li Frenkel pairs LiCl Schottky pair Li_2O Schottky pair Li interstitial with a substitutional O on the Cl site	~2 eV 1.41 eV 1.60 eV 1.67 eV	Anti-perovskite Li_3OCl DFT calculations	[2]
Li Frenkel Li_2O Schottky	0.76 3.59	NASICON-type $LiTi_2(PO_4)_3$ Classical MD	[3]
Li Frenkel Ge/P antisite (isolated) Ge/P antisite (cluster) Li_2O Schottky	0.75 2.01 1.26 3.10	NASICON-type $LiGe_2(PO_4)_3$ Classical MD	[4]
Li Frenkel Li/La antisite (cluster) Li_2O Schottky	< 1 eV	Garnet-type $Li_7La_3Zr_2O_{12}$ DFT	[5]
Li Frenkel Li_2O Schottky Li/M antisite	3.73 9.20 0.84 (Ni)	DFT/classical MD $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$	[6]
Li Frenkel	1.76	$LiMn_2O_4$	[7]
Li Frenkel Li_2O Schottky	2.15 6.33	$LiFePO_4$	[8]

Li/M antisite	1.13		
Li Frenkel	1.97	$LiMnPO_4$	[9]
Li_2O Schottky	7.36		
Li/M antisite	1.48		
Li Frenkel	1.21	$Li_2FeP_2O_7$	[10]
Li/M antisite	0.22		

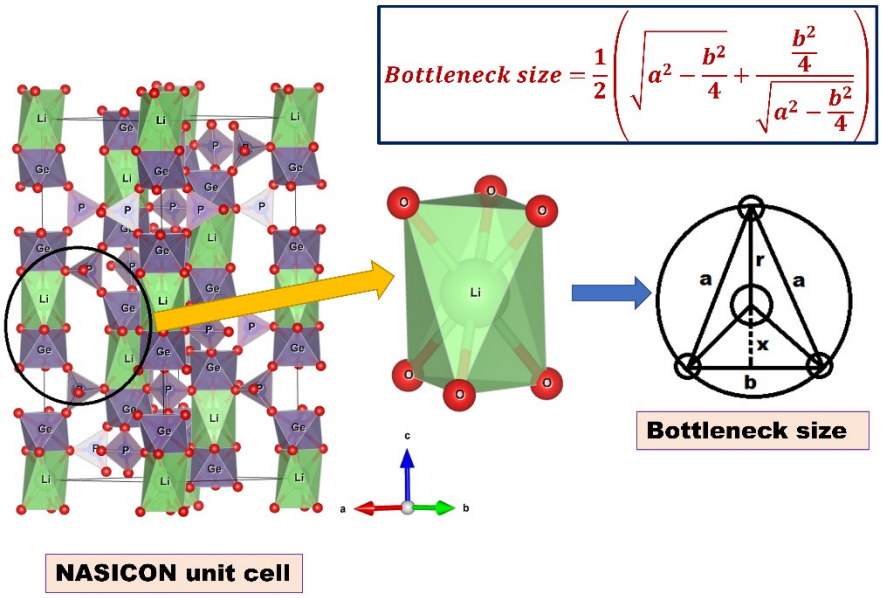


Fig. SI3: A schematic description of the bottleneck size calculation

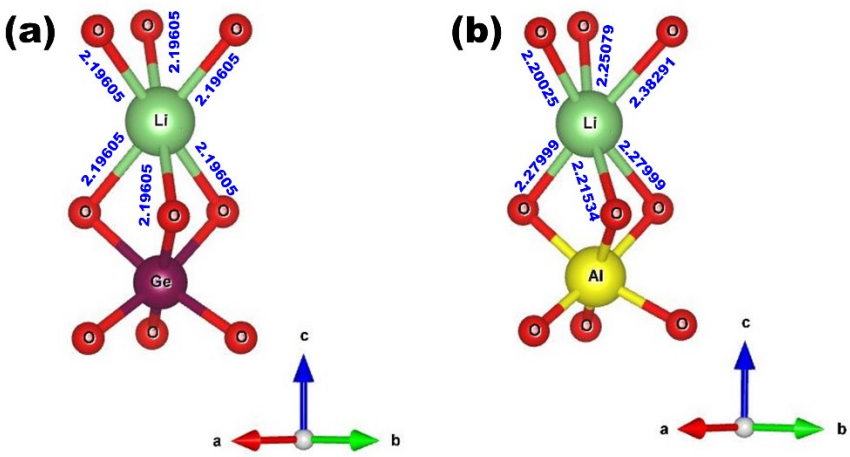
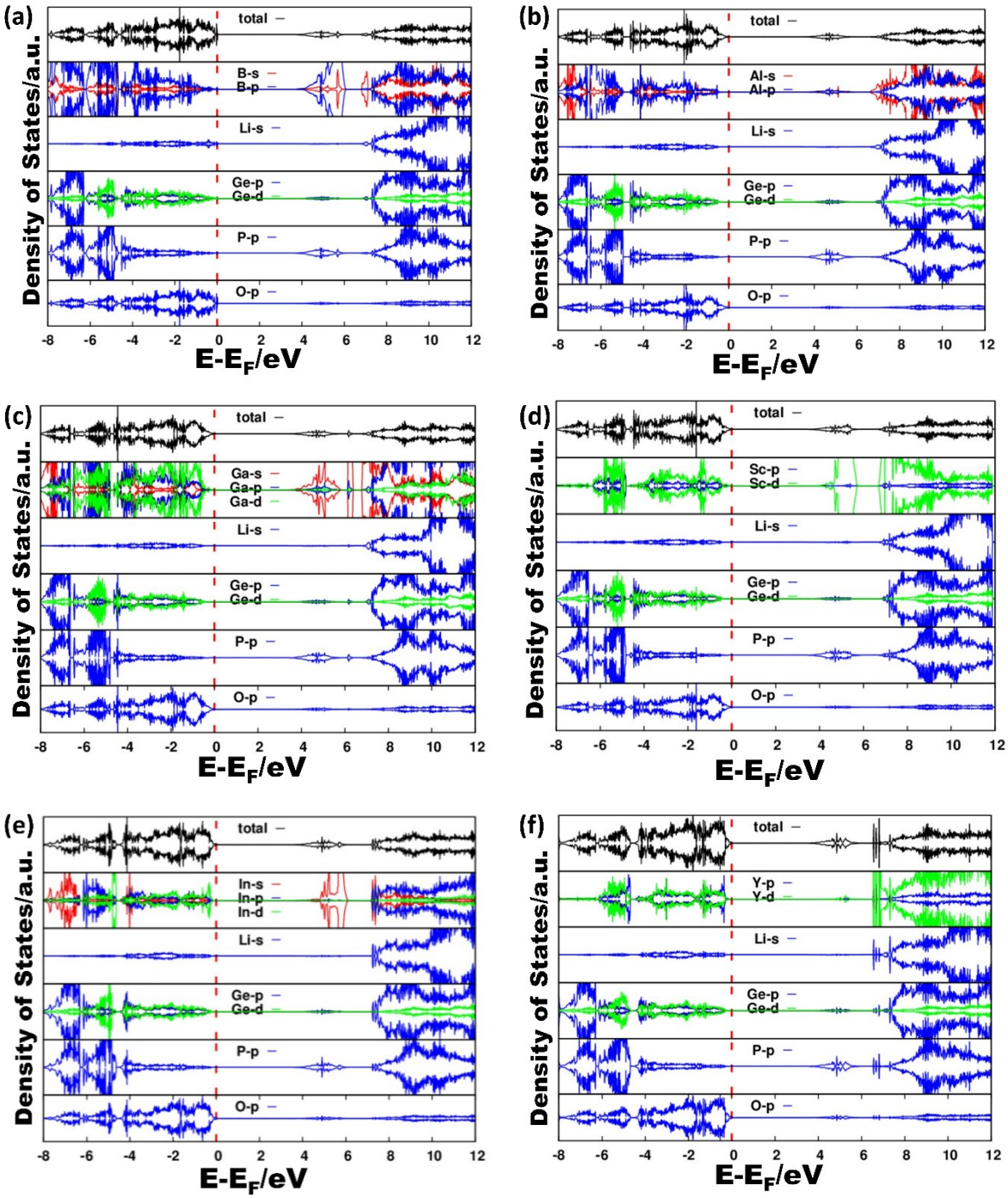


Fig. SI4: LiO_6 and Ge/AlO_6 polyhedra taken from optimized unit cell of (a) before and (b) after substitution of Al^{3+} at Ge^{4+} position. The values of Li-O bond lengths are shown.



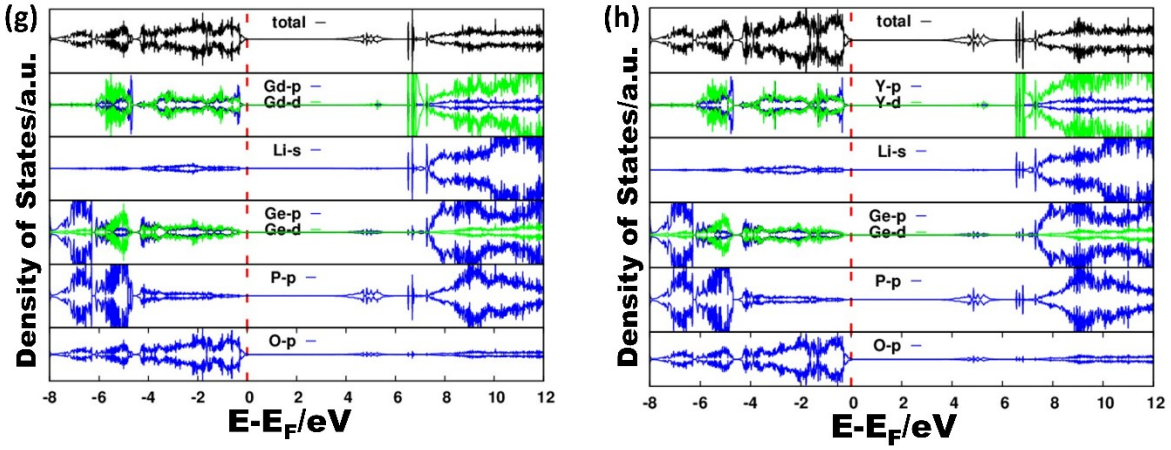


Fig. SI5: Total and atom-projected partial density of states (DOS) for (a) B^{3+}, (b) Al^{3+}, (c) Ga^{3+}, (d) Sc^{3+}, (e) In^{3+}, (f) Y^{3+}, (g) Gd^{3+} and (h) La^{3+}

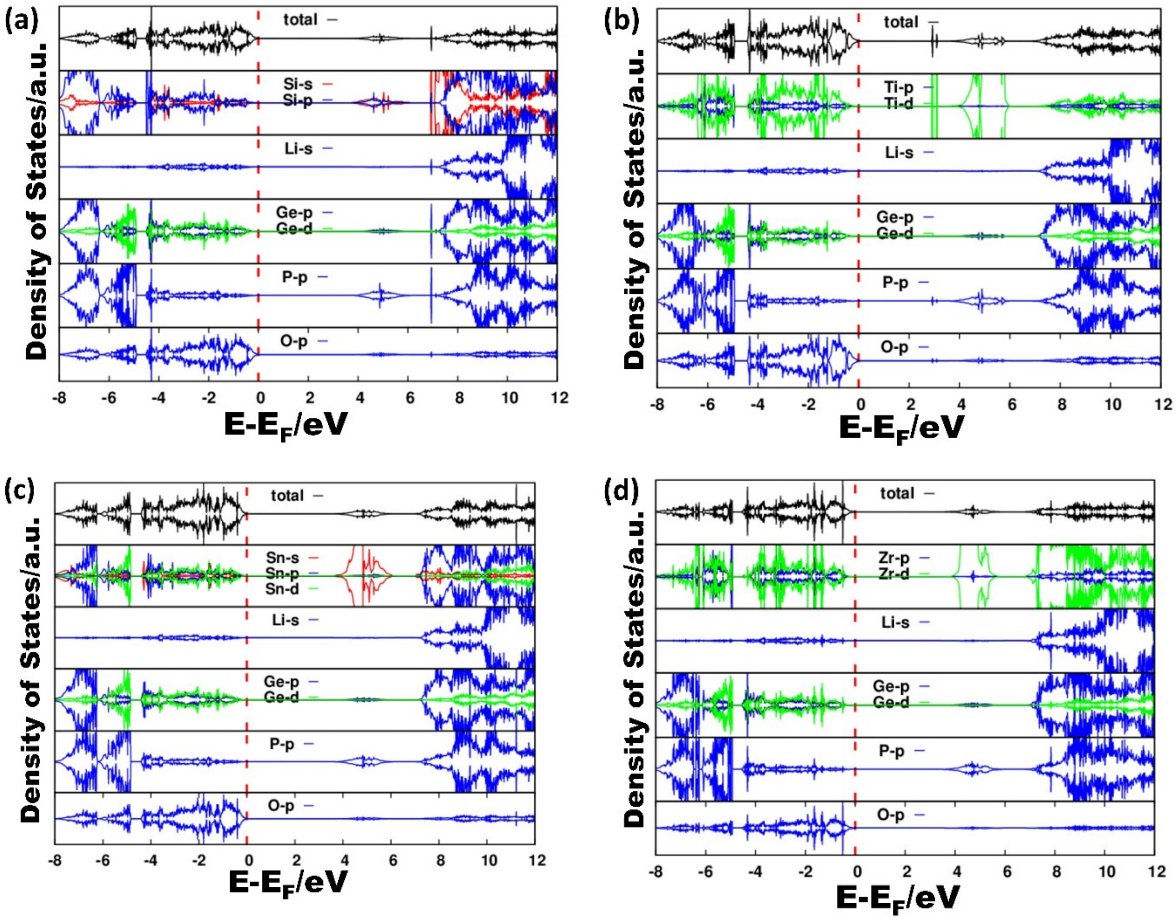


Fig. SI6: Total and atom-projected partial density of states (DOS) for (a) Si^{4+}, (b)Ti^{4+}, (c) Sn^{4+} and (d) Zr^{4+}

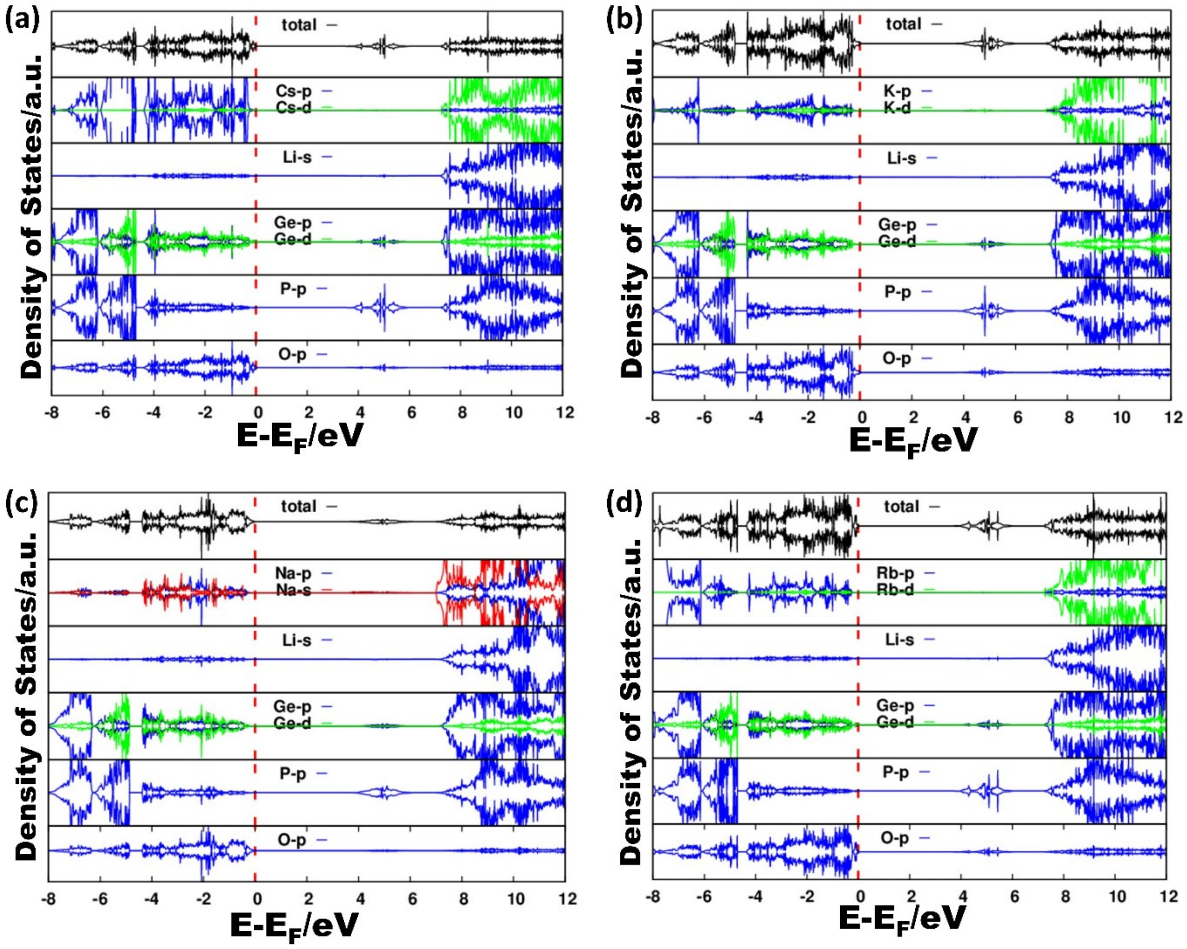
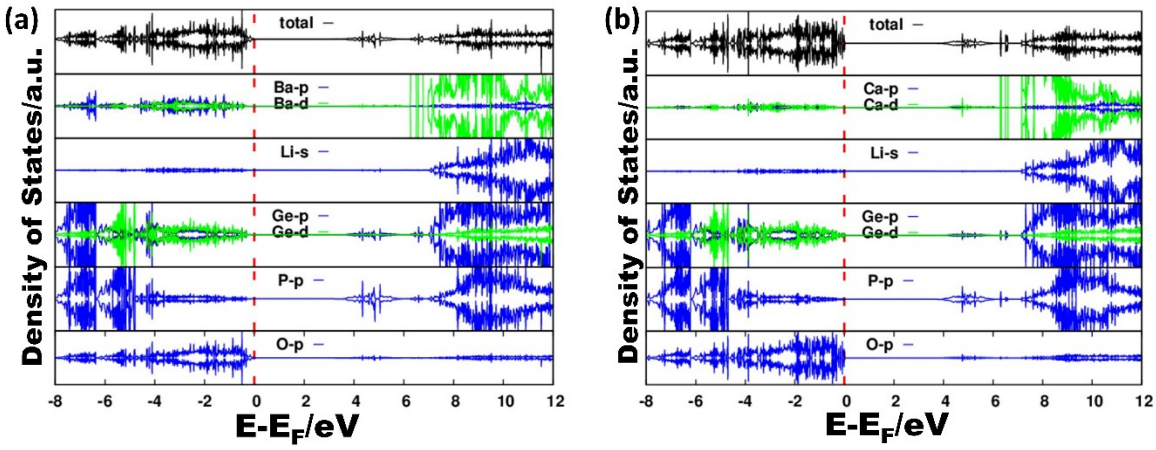


Fig. SI7: Total and atom-projected partial density of states (DOS) for (a) Cs^+, (b) K^+, (c) Na^+ and (d) Rb^+



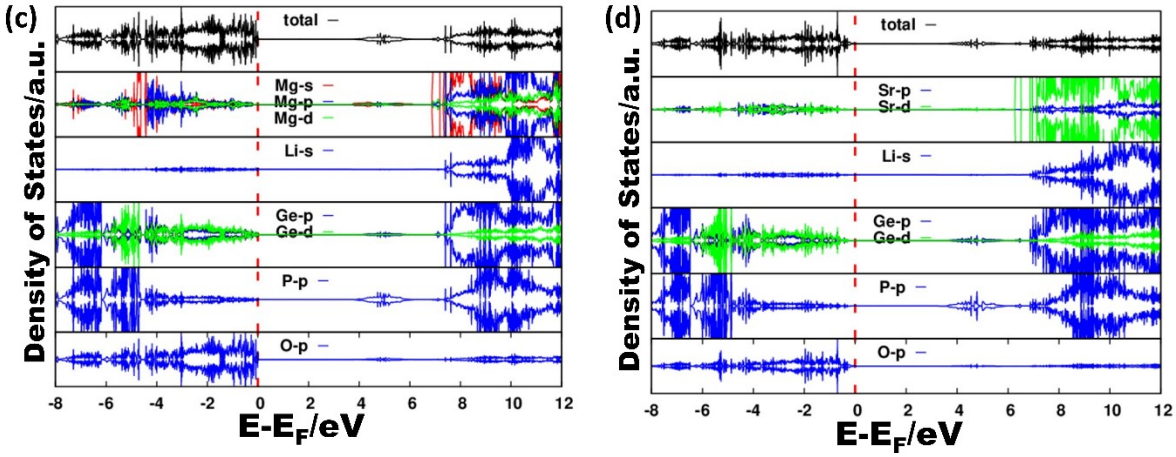


Fig. SI8: Total and atom-projected partial density of states (DOS) for (a) Ba^{2+}, (b) Ca^{2+}, (c) Mg^{2+} and (d) Sr^{2+}

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