Role of Na^+ Interstitials and Dopants in Enhancing the Na^+ Conductivity of the Cubic Na_3PS_4 Superionic Conductor

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Table S1: Average site occupancies for pristine t-Na_3PS_4, pristine and doped c-Na_3PS_4 compounds with different dopant concentrations x at 800K. To compare with the case of c-Na_3PS_4, we artificially label the Na sites in t-Na_3PS_4 as Na1, whereas the middle points between any two neighboring Na sites are labeled as Na2.

	Structures	x	Na1 site occupancy	Na2 site occupancy
t-Na_3PS_4	pristine		0.88	0.06
c-Na_3PS_4	pristine		0.84	0.08
	Na^+ excess		0.68	0.17
	Si-doped	0.0625	0.76	0.13
	Ge-doped	0.0625	0.62	0.20
	Sn-doped	0.0625	0.79	0.12

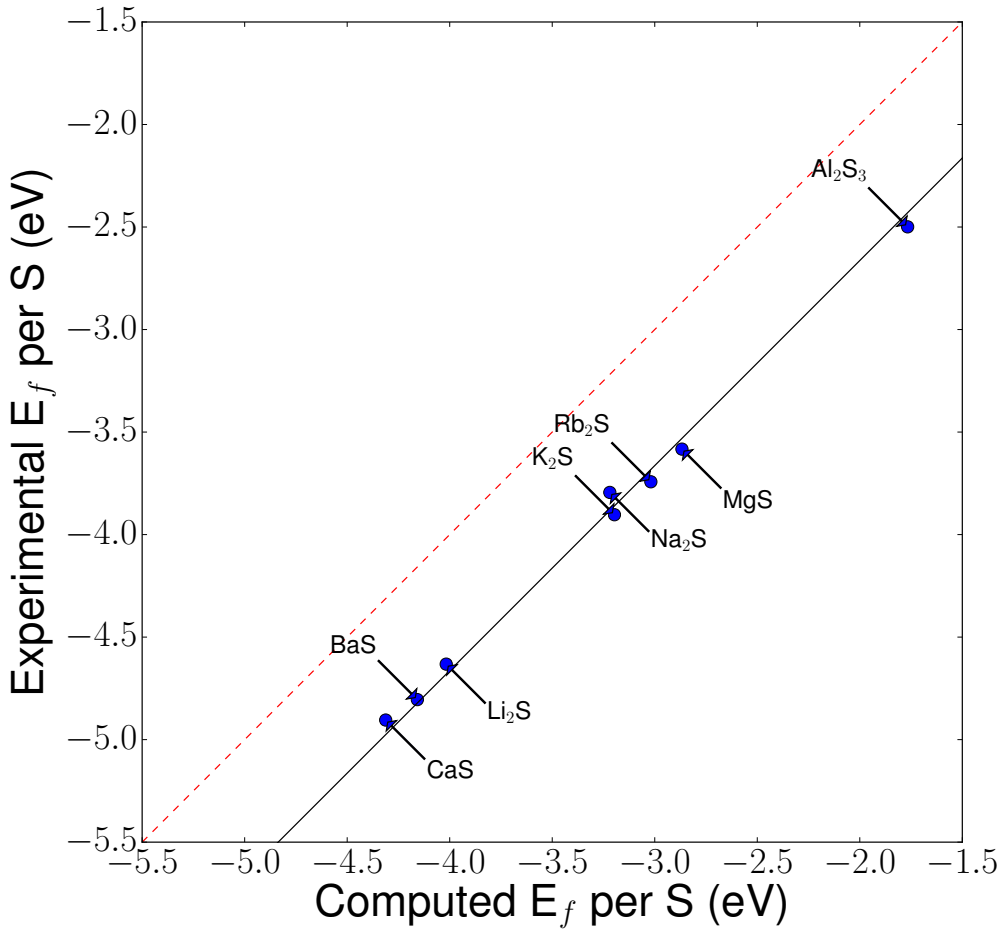
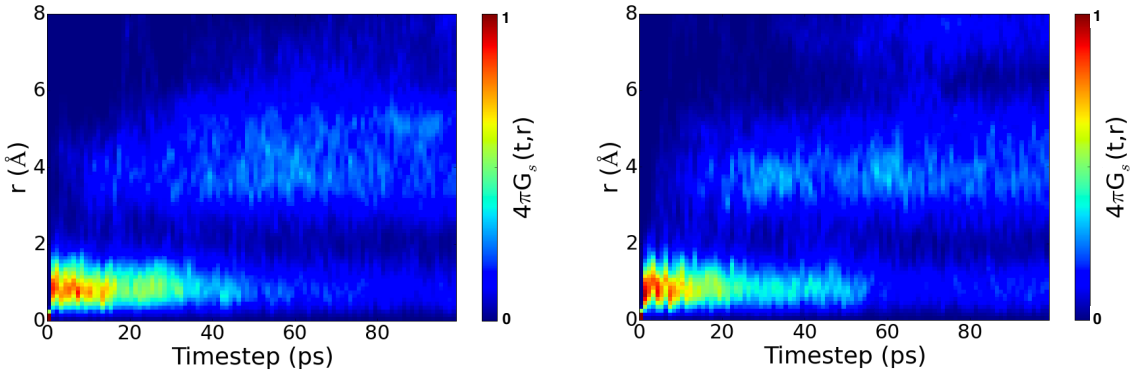


Figure S1: (Color online) Determination of energy difference constant (0.66 eV per S atom) between the DFT and experimental formation energies for sulfides.



(a) M=Si, x=0.0625

(b) M=Ge, x=0.0625

(c) M=Sn, x=0.0625

(d) M=Si, x=0.125

Figure S2: (Color online) Plots of the self-part of the van Hove correlation function (G_s) for $Na_{3+x}M_xP_{1-x}S_4$ at 800 K. G_s is a function of the Na-Na pair distance r and time t.