Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Supporting Information for

"Metal-to-insulator transition in $SmNiO_3$ induced by chemical doping: a first principles study"

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Table S1. Breathing mode for orthorhombic $SmNiO_3$ (O-SNO, Pbnm) and monoclinic $SmNiO_3$ (M-SNO, $P2_1/n$) for different magnetic configurations: T-AFM, A-AFM, FM, and PM (paramagnetic). Larger octahedron is denoted as N_L and smaller octahedron as N_S, respectively.

Magnetism	Space group	Octahedron	Octahedron volume (Å^3)	Volume N_L/N_S (%)	Bader Charge value (e)
PM	Pbnm	N_S	9.44	0.00	1.165
		N_L	9.44		1.165
	$P2_1/n$	N_S	9.57	0.04	1.190
		N_L	9.57		1.121
FM	Pbnm	N_S	9.65	0.02	1.211
		N_L	9.65		1.210
	$P2_1/n$	N_S	9.13	10.35	1.169
		N_L	10.18		1.233
T-AFM	Pbnm	N_S	9.33	0.00	1.195
		N_L	9.33		1.199
	$P2_1/n$	N_S	9.12	10.35	1.161
		N_L	10.17		1.222
A-AFM	Pbnm	N_S	9.33	0.00	1.195
		N_L	9.33		1.199
	$P2_1/n$	N_S	9.11	11.26	1.167
		N_L	10.27		1.223

Figure S1. Spin alignment in A-type antiferromagnetism (A-AFM) and T-type AFM (T-AFM). In A-AFM, two adjacent Ni layers have opposite magnetic moments along the [001] direction. On the other hand, T-AFM has more complex magnetic ordering with stairwise parallel magnetic moments.

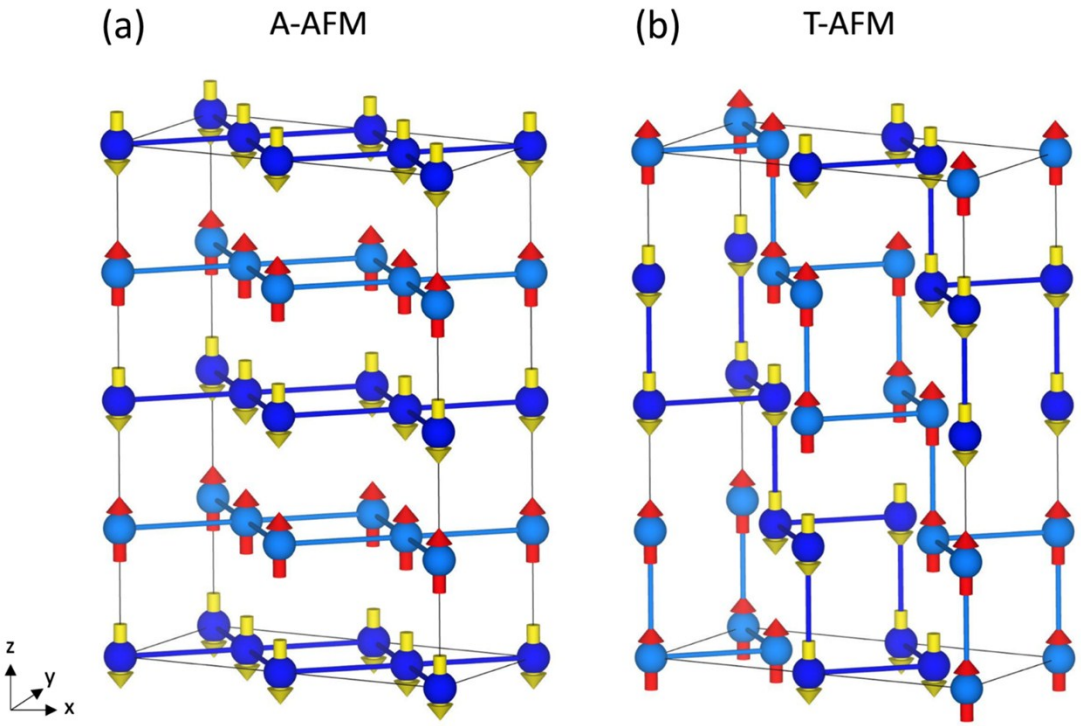

Figure S2. Total density of states (TDOS) of orthorhombic $SmNiO_3$ (O-SNO, Pbnm) and monoclinic $SmNiO_3$ (M-SNO, $P2_1/n$) by PBEsol+2: (a) T-AFM of M-SNO, (b) A-AFM of M-SNO, (c) FM of M-SNO, (d) T-AFM of O-SNO (e) A-AFM of O-SNO, and (f) FM of O-SNO.

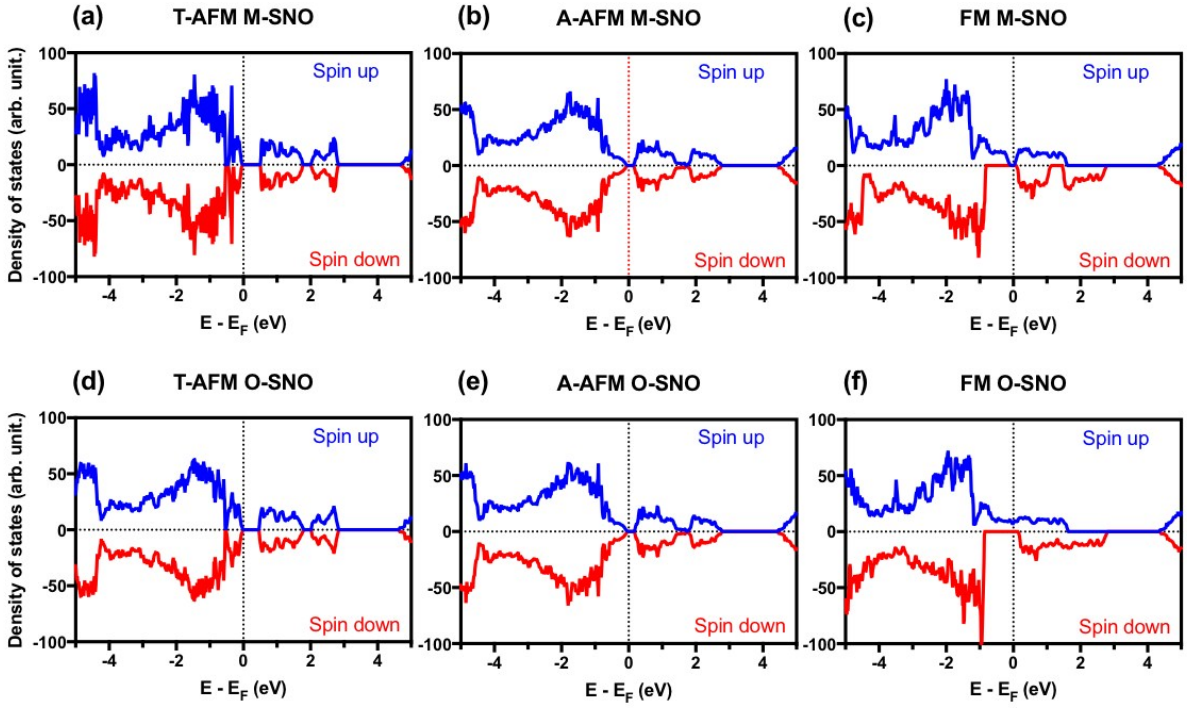

Figure S3. TDOS by SCAN functional: (a) T-AFM of M-SNO, (b) A-AFM of M-SNO, (c) FM of M-SNO, (d) T-AFM of O-SNO (e) A-AFM of O-SNO, and (f) FM of O-SNO. Except for A-AFM of O-SNO, all magnetic configurations and symmetry were predicted to be metallic.

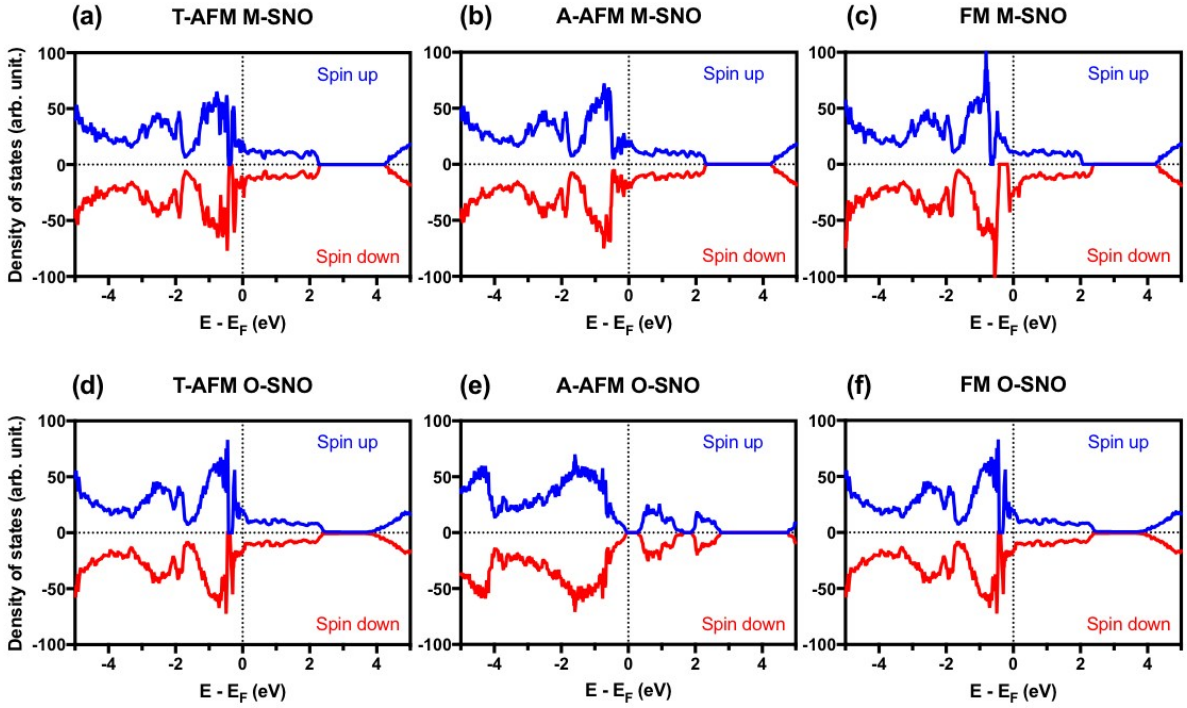

Figure S4. (a) Stable hydrogen occupation sites for Ni layer (blue) and Sm layer (yellow) in O-SNO. Several sites that are closer than 1 Å was reduced to one site. (b) Distribution of relative energy for 1 hydrogen occupying Ni or Sm layers in O-SNO.