Electronic Supplementary Information

Monolayer triphosphates MP₃ (M=Sn, Ge) with excellent basal catalytic activity for hydrogen evolution reaction

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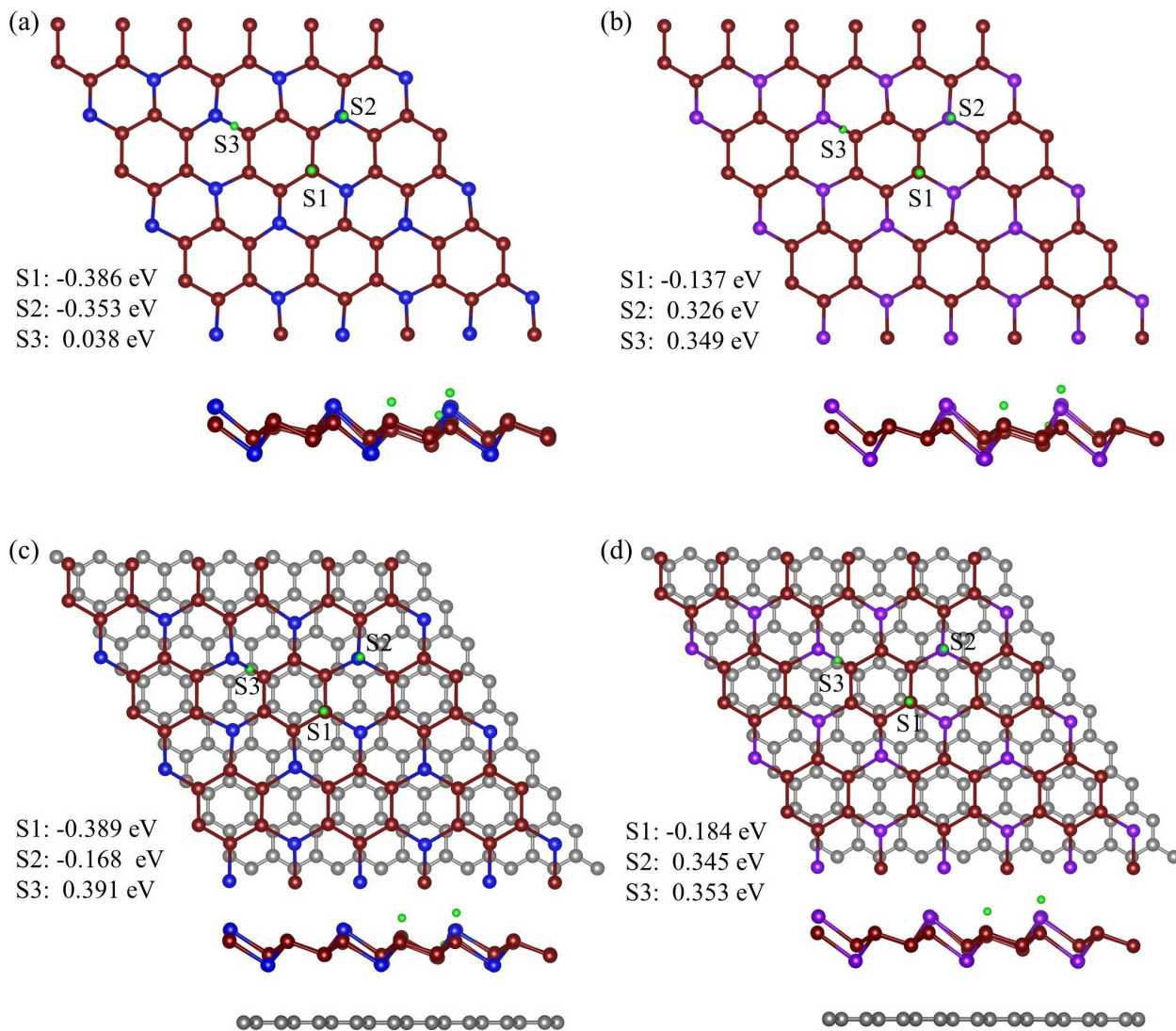[∇] Department of Physics and Materials, East China Normal University, Shanghai 200241, China

(a)

S2
S3
S1

S1: -0.386 eV
S2: -0.353 eV
S3: 0.038 eV

(b)

S2
S3
S1

S1: -0.137 eV
S2: 0.326 eV
S3: 0.349 eV

(c)

S2
S3
S1

S1: -0.389 eV
S2: -0.168 eV
S3: 0.391 eV

(d)

S2
S3
S1

S1: -0.184 eV
S2: 0.345 eV
S3: 0.353 eV

Figure S1. Top and side view of the optimized structural 4×4×1 supercell of (a) GeP$_3$ monolayer, (b) SnP$_3$ monolayer, (c) GeP$_3$@graphene, (d) SnP$_3$@graphene.

Table S1 Computed bond length, monolayer thickness and layer distance for GeP_3 and SnP_3

System	Ge (Sn)-P	P-P	P-H	thickness	layer distance
GeP_3	2.508	2.175	1.432	2.421	/
SnP_3	2.712	2.168	1.434	2.875	/
GeP_3@graphene	2.566	2.211	1.435	5.239	3.208
SnP3@graphene	2.731	2.184	1.435	5.921	3.338

Table S2. Computed adsorption energy (E_a), adsorption distance (d), charge transfer (ΔQ) of the atoms around the adsorption site

System	E_a (eV)	d (Å)	Bader charge of hydrogen atom	ΔQ (e)
GeP$_3$	-0.386	1.431	1.319	0.319
GeP$_3$@graphene	-0.389	1.434	1.351	0.351
SnP$_3$	-0.137	1.433	1.312	0.312
SnP$_3$@graphene	-0.185	1.434	1.379	0.379
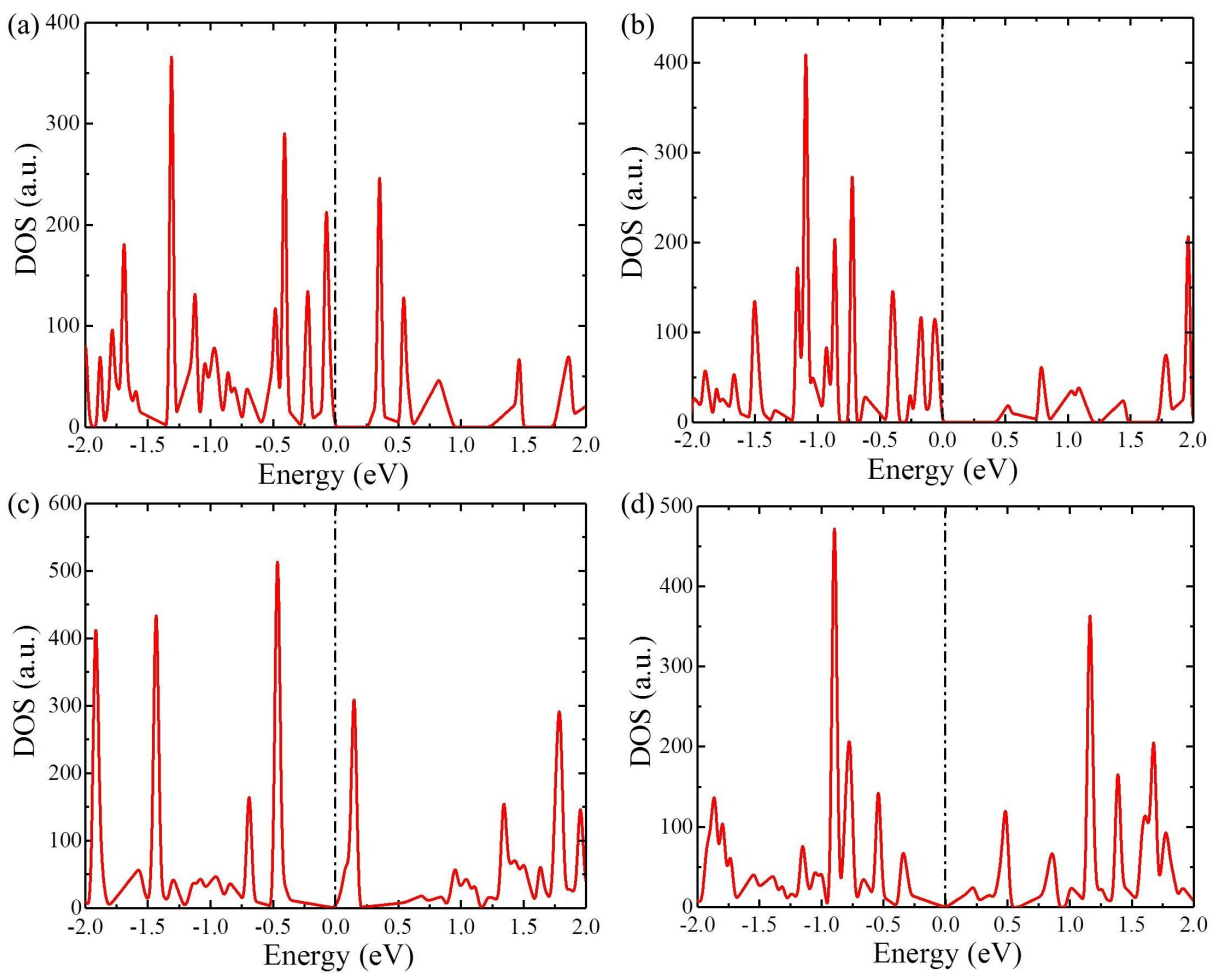
Figure S2. Density of states computed based on the PBE functional for (a) GeP$_3$ monolayer, (b) SnP$_3$ monolayer, (c) GeP$_3$@graphene heterobilayer, and (d) SnP$_3$@graphene heterobilayer.
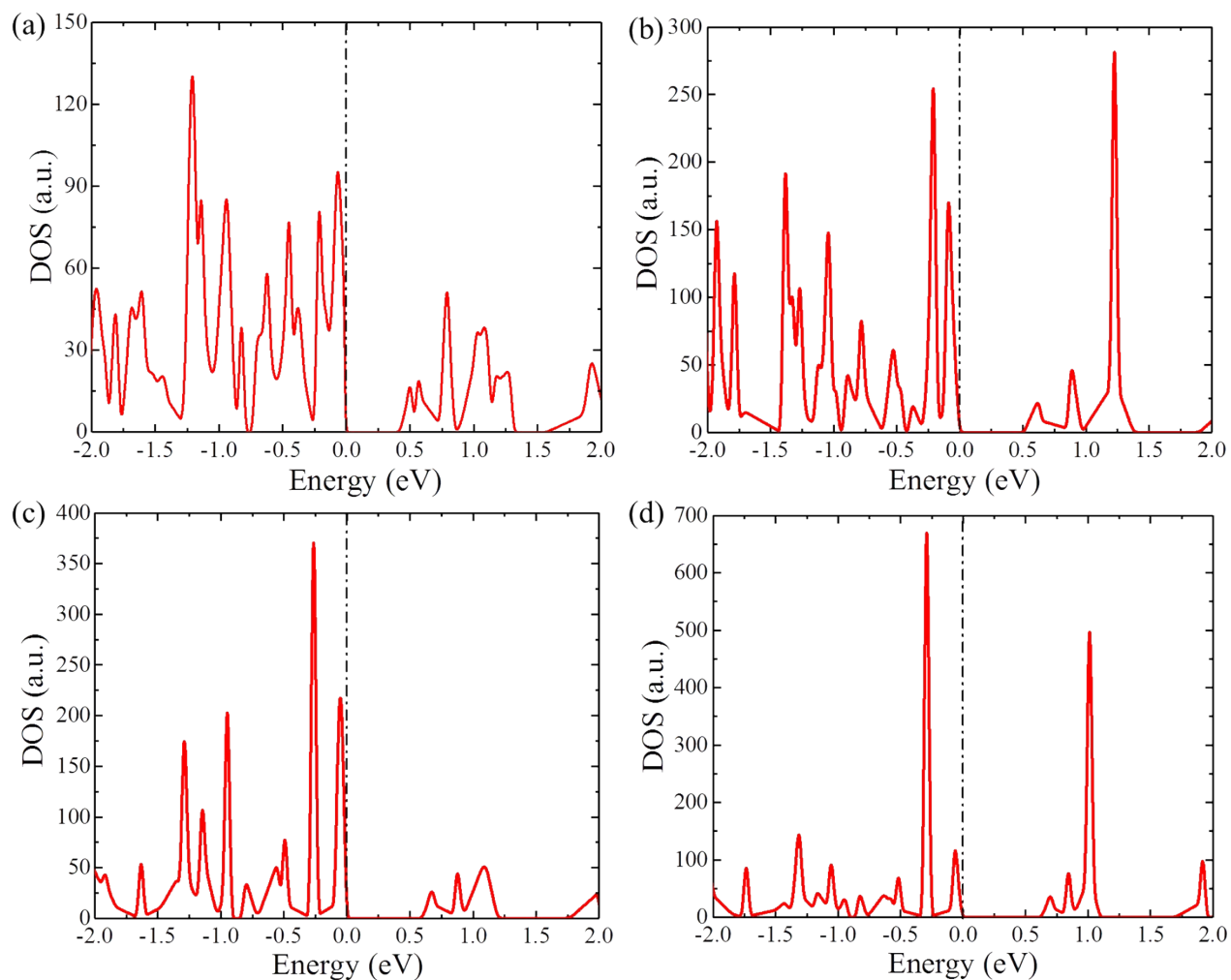
Figure S3. Effect of biaxial strain (a) -0.02, (b) -0.01, (c) 0.01, (d) 0.02 on the density of states of GeP$_3$ monolayer, based on HSE06 computation.
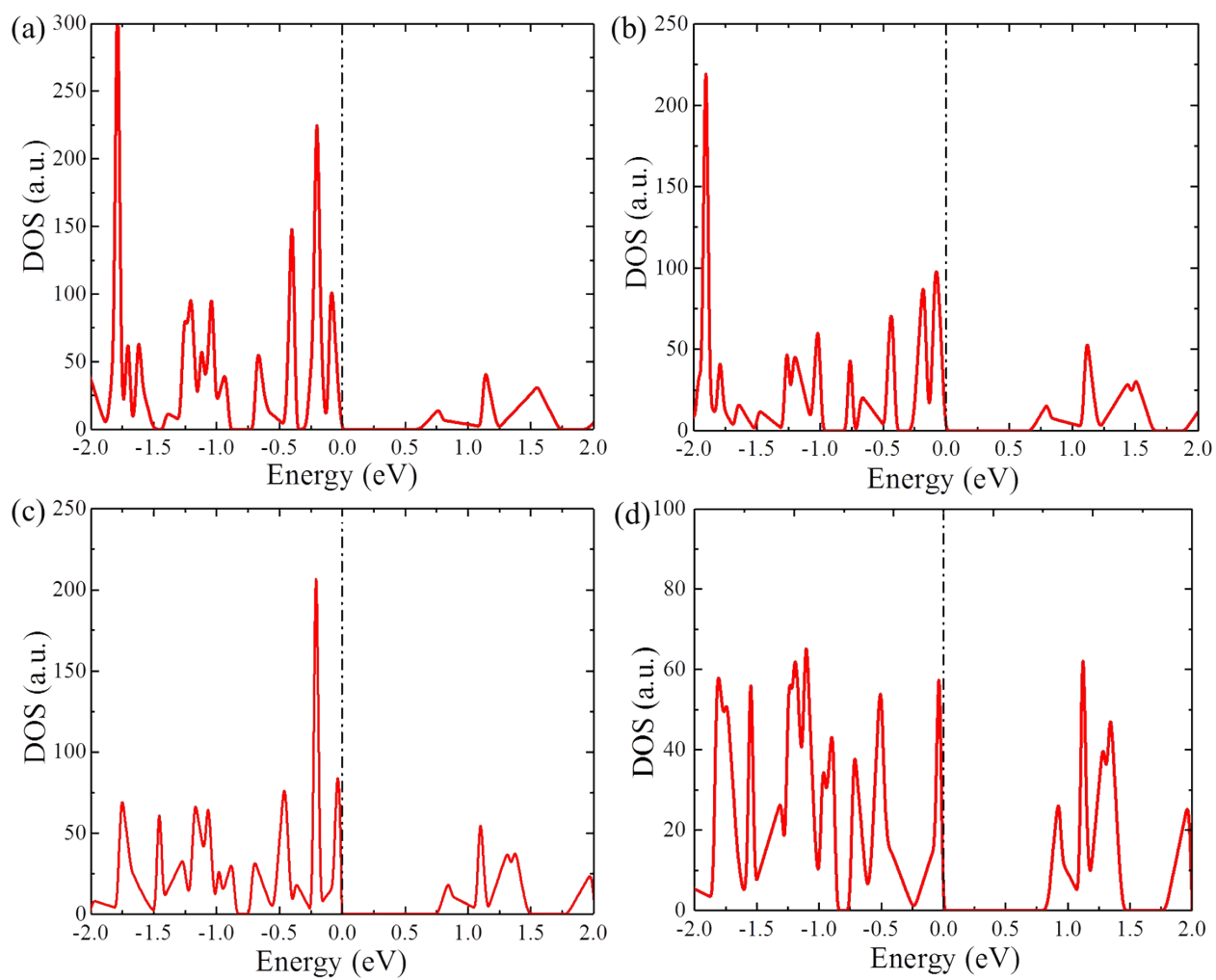
Figure S4. Effect of biaxial strain (a) -0.02, (b) -0.01, (c) 0.01, (d) 0.02 on the density of states of SnP$_3$ monolayer, based on HSE06 computation.
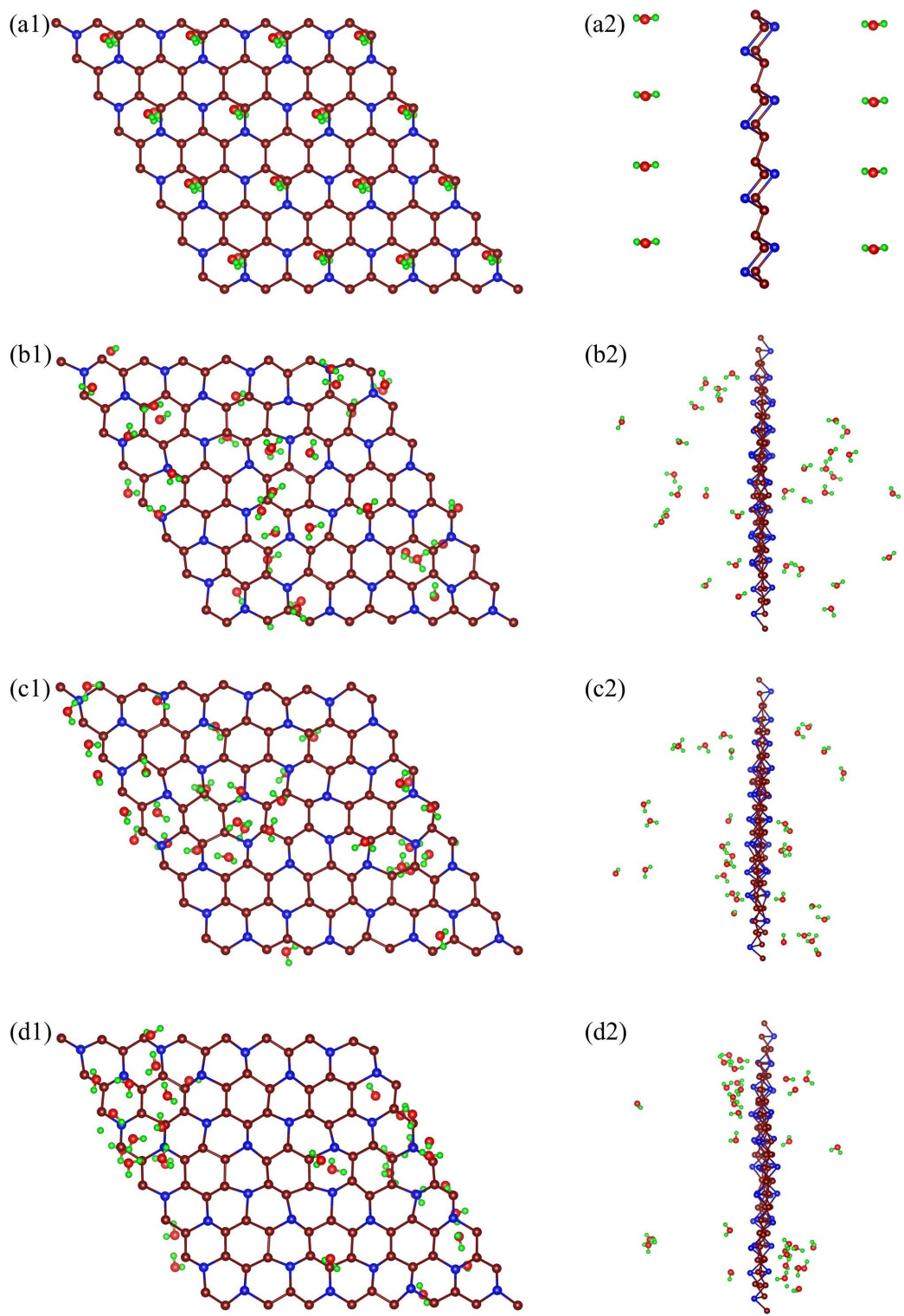
Figure S5. Ab initio MD simulation results of the 6×6×1 GeP$_3$ monolayer supercell with 32 water molecules at the simulation time (a1)-(a2) 0 fs, (b1)-(b2) 1000 fs, (c1)-(c2) 3000 fs, (d1)-(d2) 6000 fs from top and side view, respectively. The temperature is controlled at 300 K.
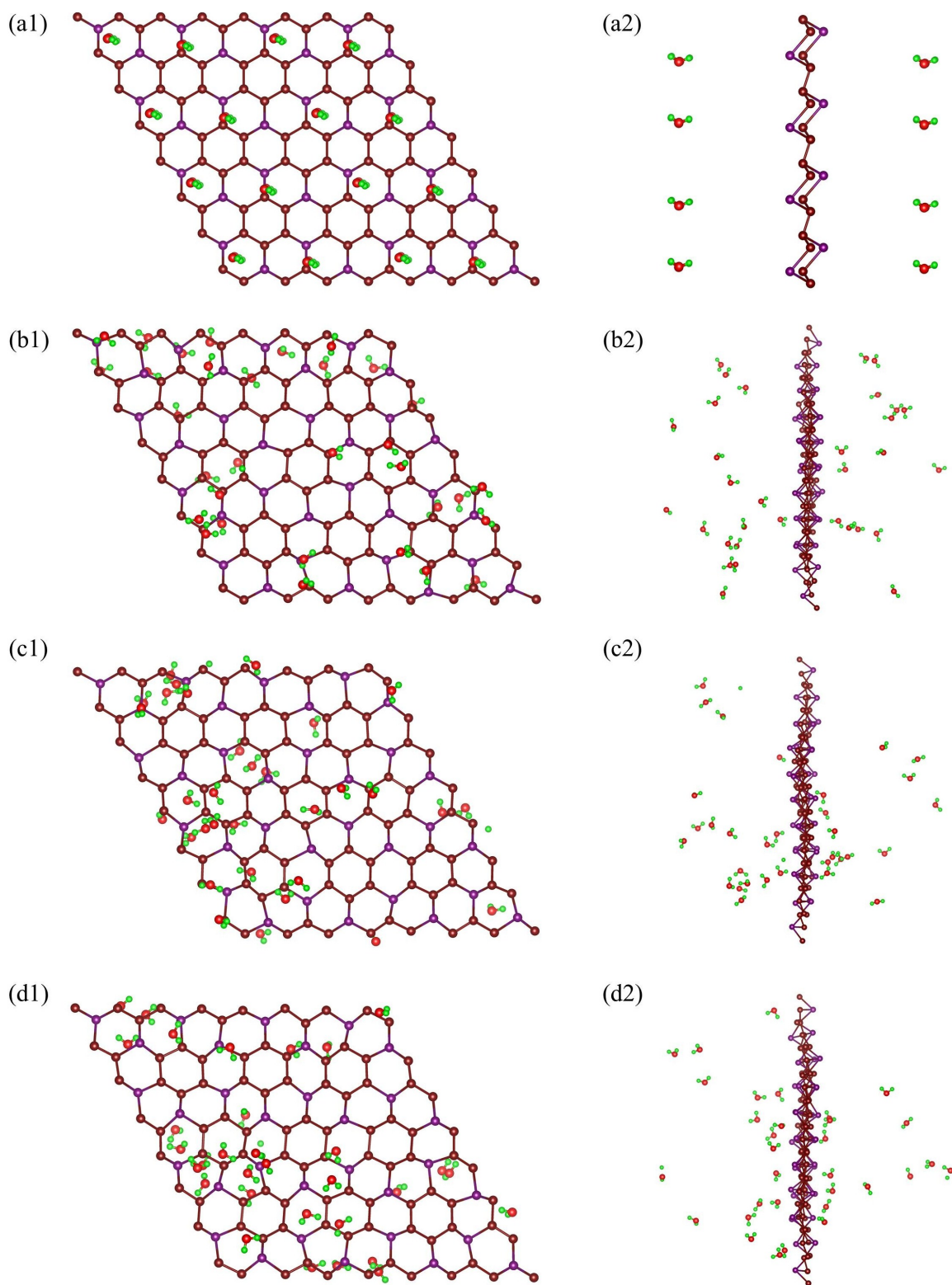
Figure S6. Ab initio MD simulation results of the 6×6×1 SnP$_3$ monolayer supercell with 32 water molecules at the simulation time (a1)-(a2) 0 fs, (b1)-(b2) 1000 fs, (c1)-(c2) 3000 fs, (d1)-(d2) 6000 fs from top and side view, respectively. The temperature is controlled at 300 K.