Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

Tunable electronic and optical properties in bucking one-atom-thin non-lamellar B_3S monolayer

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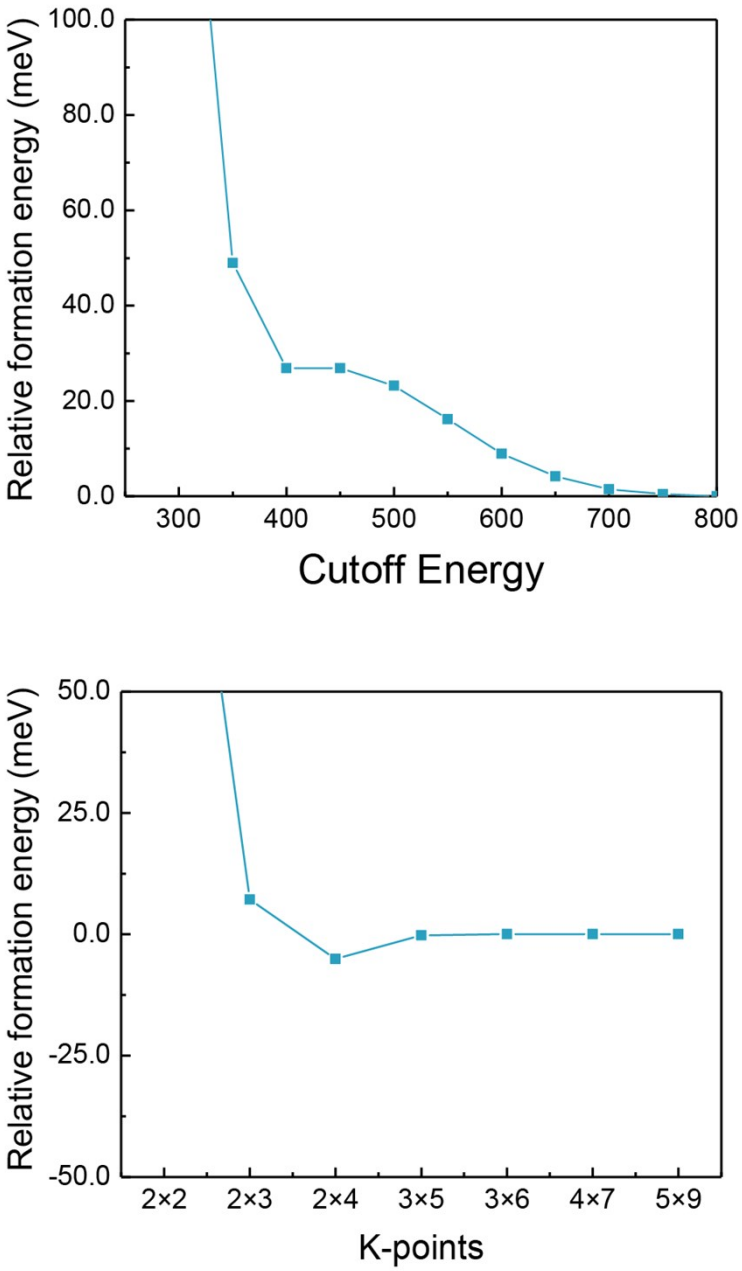

Fig. S1. The convergence test with respect to cutoff energy and K-point mesh of the h1-B_3S monolayer using an orthogonal supercell.

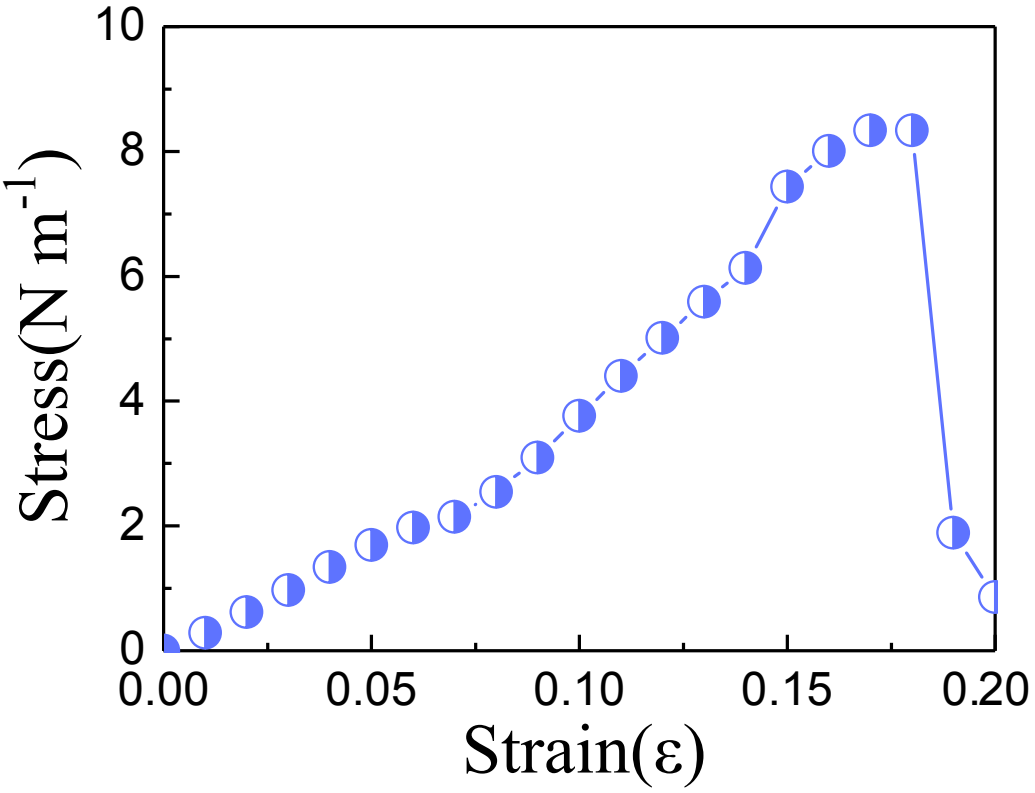

Fig. S2. The stress-strain diagram of the h1-B3S monolayer.

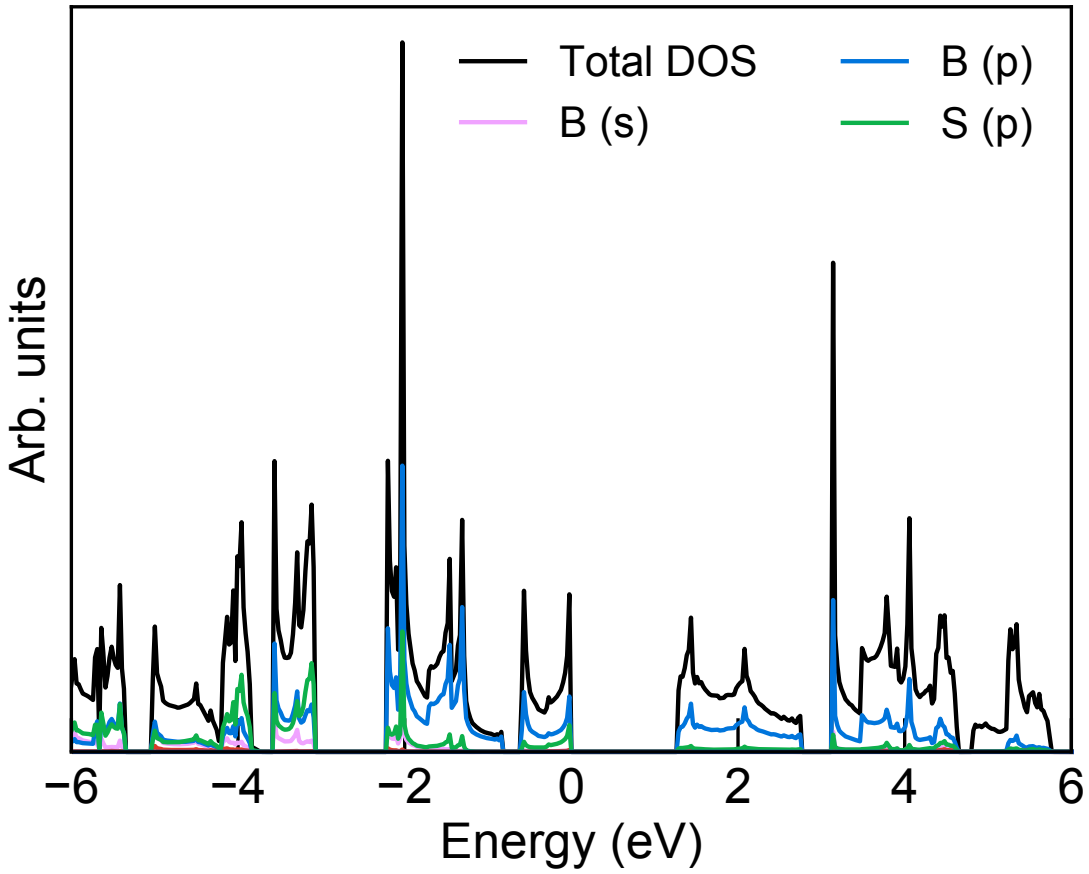

Fig. S3. Total and orbital projected DOS of the h1-B3S monolayer.

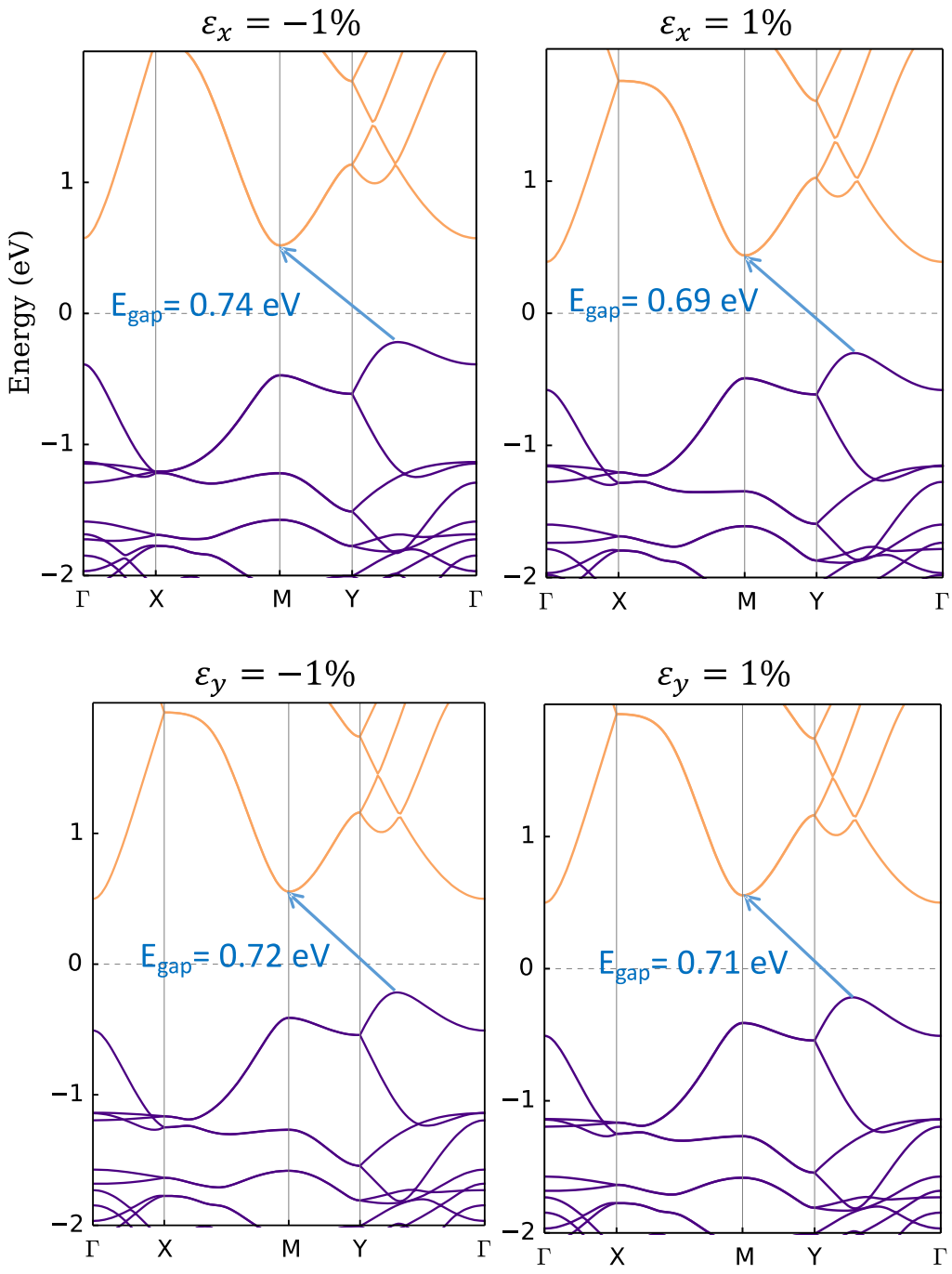

Fig. S4. Band structures of oxidized B_3S monolayer under uniaxial strains.

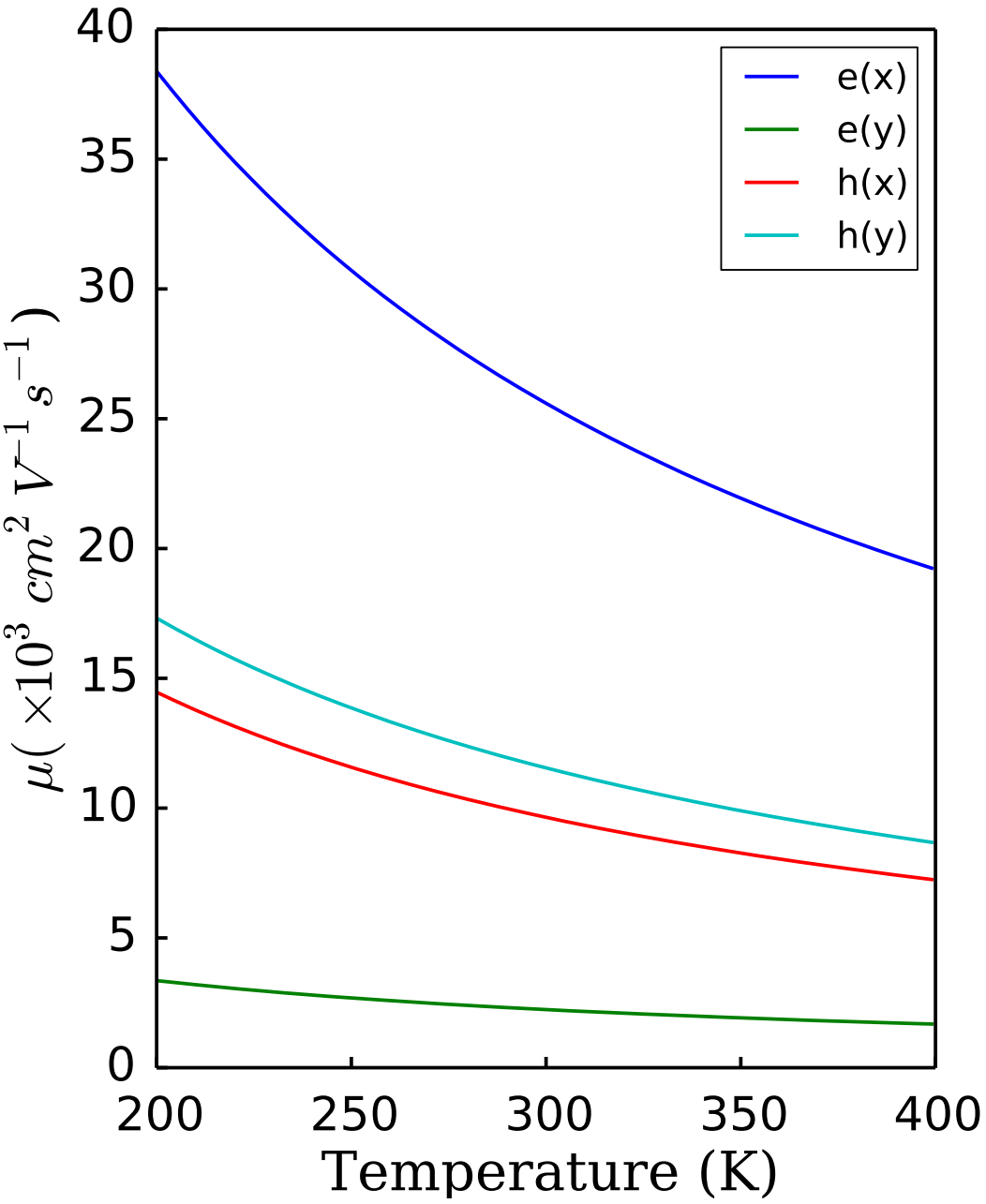

Fig. S5. Temperature dependent carrier mobilities along x and y directions.

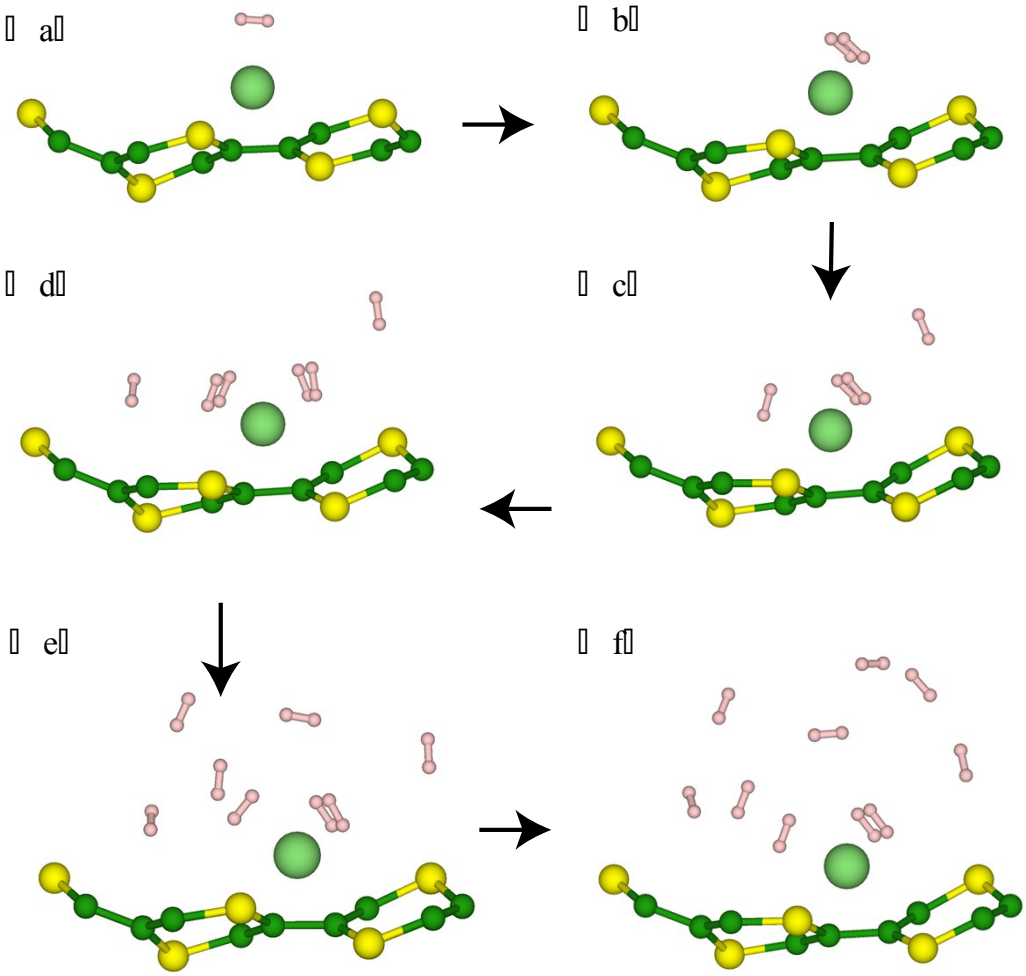

Fig. S6. Atomic configurations of H_2 adsorbed on Li-decorated h1-B_3S monolayer.

Table S1. Atomic configuration and adsorption energies of fully oxidized h1-B_3S using pure PBE and PBE plus various vdW correction methods.

vdW method	Lattice constant (Å)	S-O bond length (Å)	E_{ads-O} (eV)
Pure PBE	5.669	1.484	-0.34
PBE+D2	5.661	1.483	-0.37
PBE+TS	5.637	1.483	-0.43
PBE+TS+SCS	5.644	1.485	-0.38