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

Supporting Information

Semiconductor Sc_2S_3 monolayer with ultrahigh carrier mobility and UV blocking filter application

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1. Details of structure prediction

The particle swarm optimization (PSO) method within the evolutionary algorithm as implemented in the CALYPSO code was employed to find the lowest energy structures of 2D Sc_xS_{1-x} ($0<x<1$) monolayer. The unit cells containing 1, 2, 3, and 4 formula units (f.u.) were considered. In the first step, random structures with certain symmetry are constructed in which atomic coordinates are generated by the 2D crystallographic symmetry operations. Local optimizations using the VASP code were done with the conjugate gradients method and stopped when Gibbs free energy changes became smaller than 1×10^{-5} eV per cell. After processing the first generation structures, 60% of them with lower Gibbs free energies are selected to construct the next generation structures by PSO. 40% of the structures in the new generation are randomly generated. A structure fingerprinting technique of bond characterization matrix is applied to the generated structures, so that identical structures are strictly forbidden. These procedures significantly enhance the diversity of the structures, which is crucial for structural global search efficiency. In most cases, structural searching simulations for each calculation were stopped after generating 1000 ~ 1200 structures (e.g., about 20 ~ 35 generations).

2. The related graphs of discussions in the paper

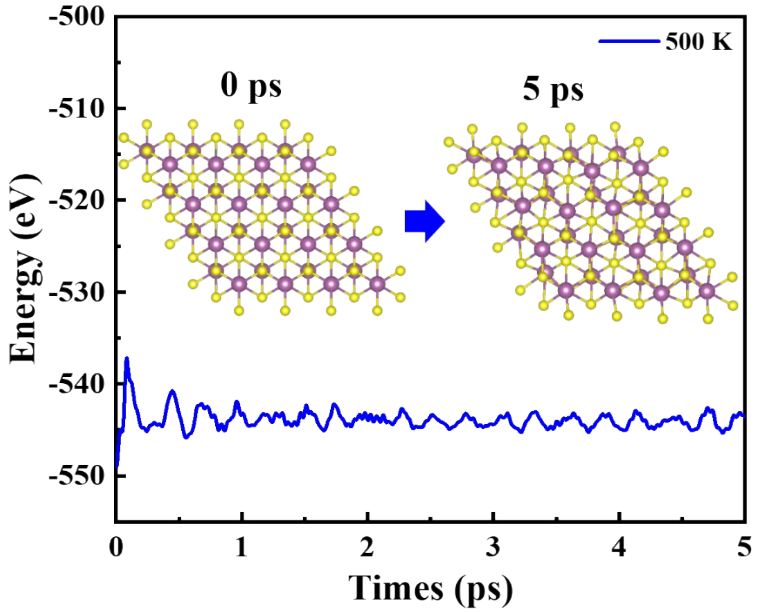


Figure S1. Snapshot of the final frame of the Sc_2S_3 monolayer at 500K of MD simulation.

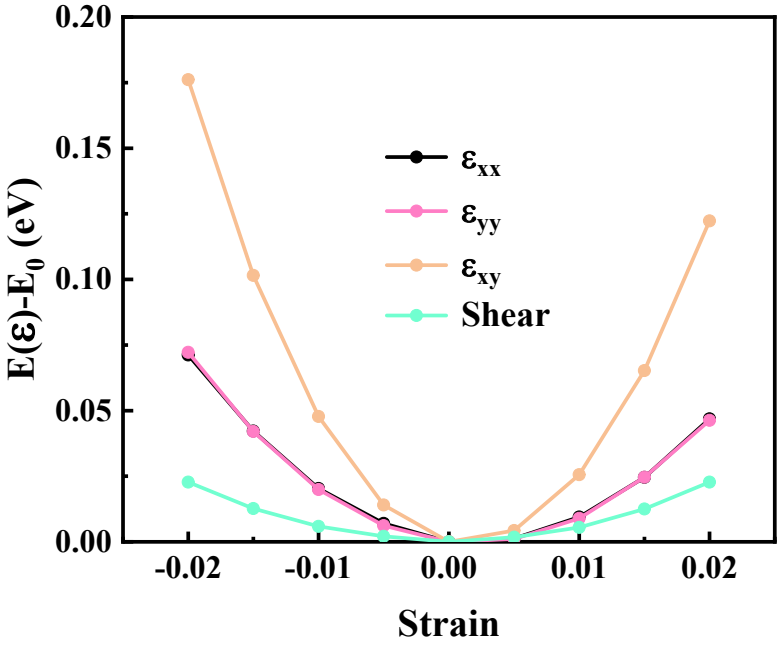


Figure S2. Energy variation curves of Sc_2S_3 monolayer with uniaxial, biaxial, and shear strain.

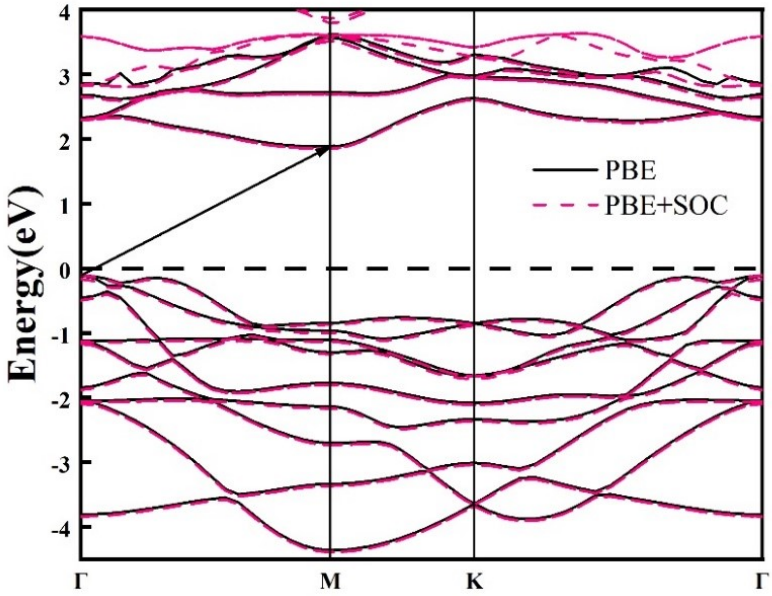
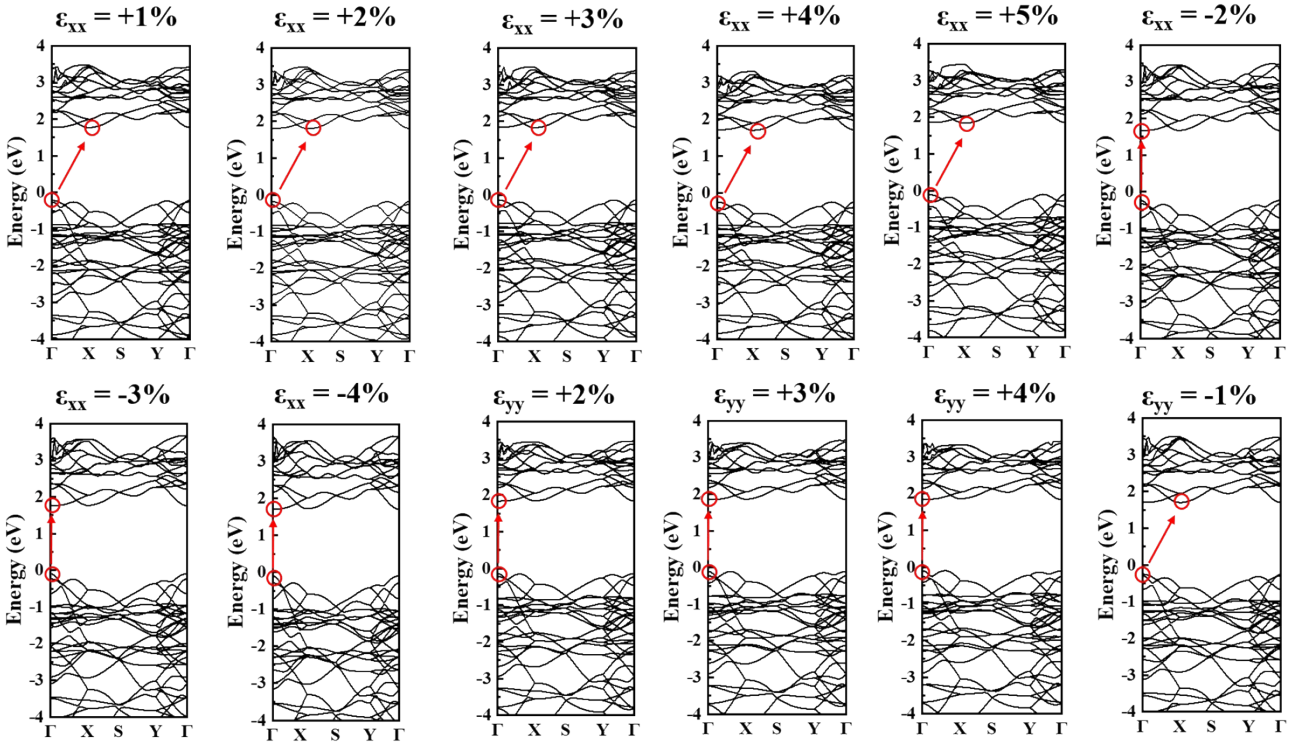


Figure S3. The band structures of Sc_2S_3 monolayer based on PBE and PBE+SOC.



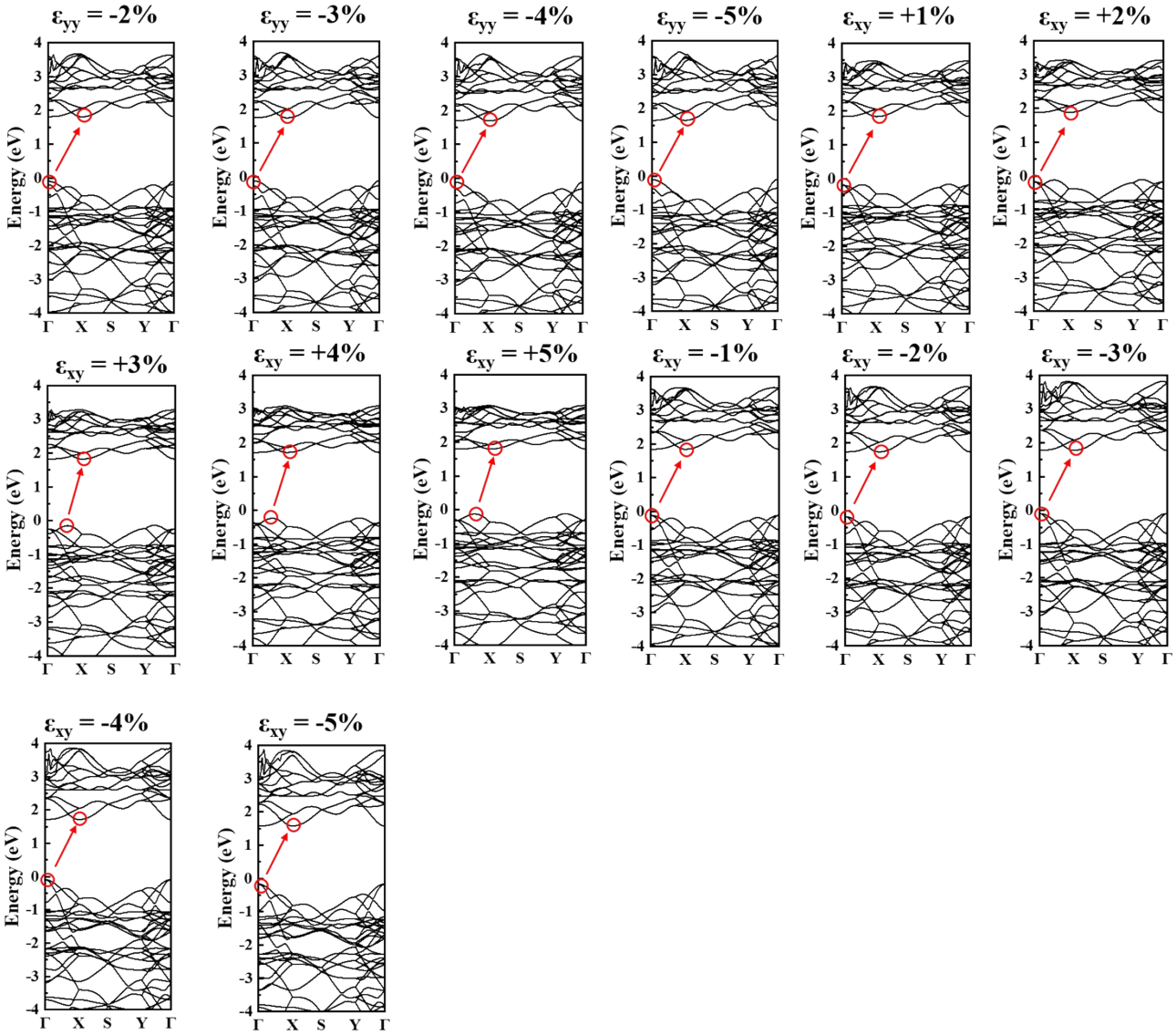


Figure S4. Dependence of band gaps under biaxial and uniaxial strain (-5%~5%) for Sc_2S_3 monolayer.

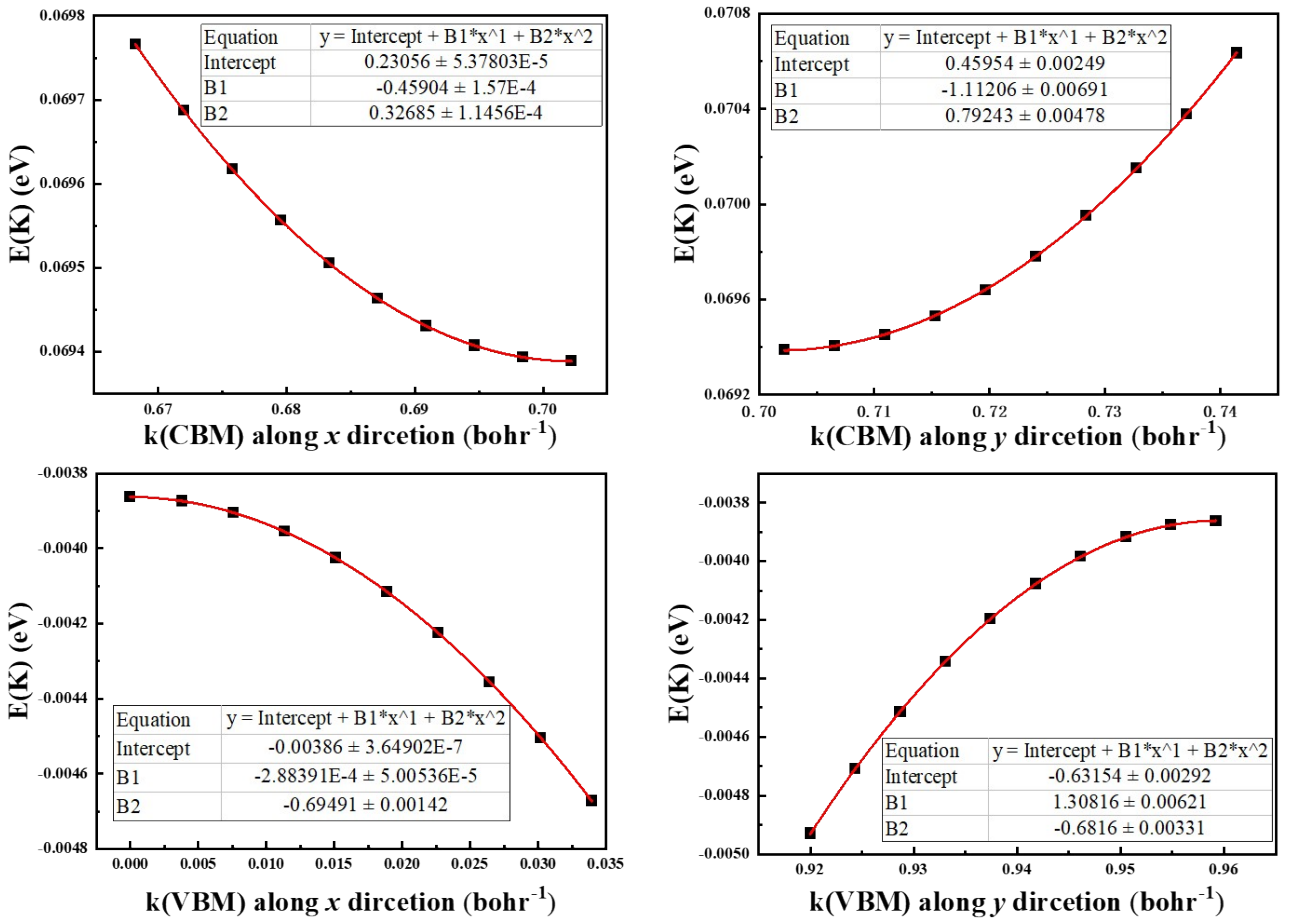


Figure S5. The fitted curves of E(k)-k of Sc_2S_3, where E(k) is the energy of k states around the conduction band minimum (CBM) or valence band maximum (VBM) in the first Brillouin zone, for calculate the corresponding effective masses.

Table S1 Structural information of the predicted Sc_2S_3 monolayer

Phase	Space Group	Lattice Parameters (Å, °)	Positions				Charge (|e|)
			Atoms	*x*	*y*	*z*	
Sc_2S_3	*P*-3*m*1	$a = b = 3.73$ $\alpha = \beta = 90$ $\gamma = 120$	Sc1	0.66667	0.33333	0.55879	-1.77
			Sc2	0.33333	0.66667	0.44121	-1.77
			S1	0.66667	0.33333	0.39896	1.09
			S2	0.33333	0.66667	0.60104	1.09
			S3	0.00000	0.00000	0.50000	1.35