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

Giant anisotropic photogalvanic effect in flexible AsSb monolayer with ultrahigh carrier mobility

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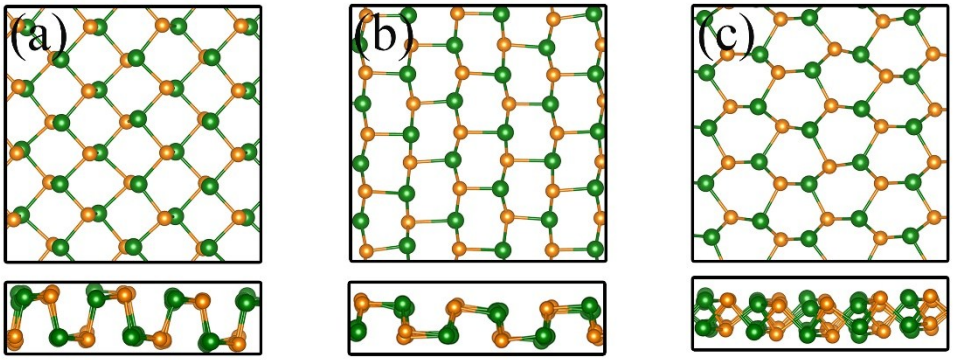
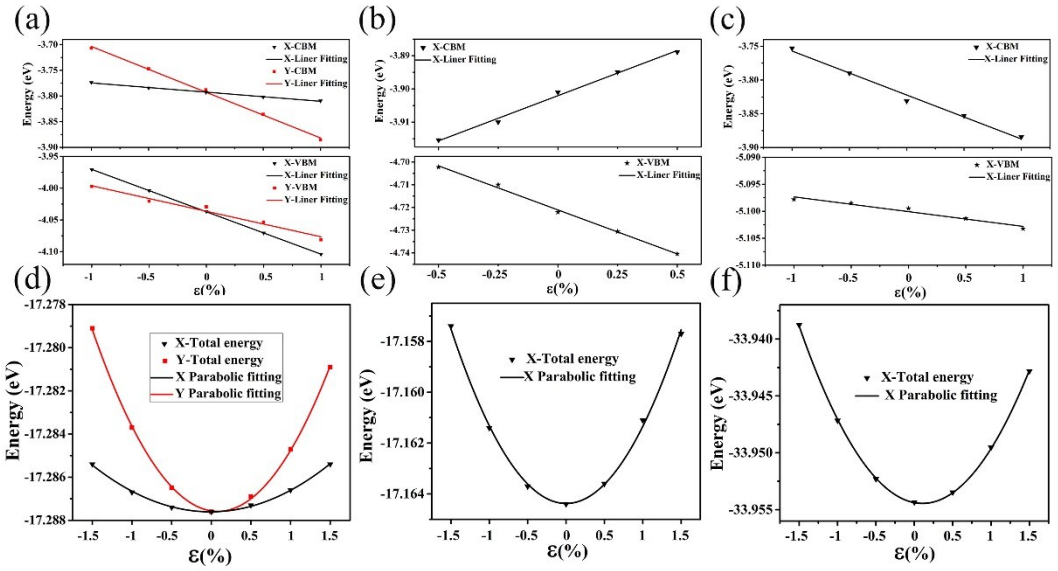
Tables S1. Optimized structural parameters and of AsSb allotropes (as shown in Figure 1) at the PBE theoretical level.

Phase	Lattice Constant (Å)		Bond length (Å)			Angle (°)		Formation energy (eV/atom)
	a	b	d_1	d_2	d_3	θ_1	θ_2	
α-AsSb	4.75	4.04	2.67	2.72	—	97.30	98.34	-2.78
γ-AsSb	6.24	3.85	2.68	2.78	—	97.43	97.33	-2.75
ε-AsSb	6.78	7.23	2.67	2.72	2.72	83.49	99.34	-2.70



Figures S1. Top and side views of (a) α-AsSb, (b) γ-AsSb and (c) ε-AsSb monolayer snapshotted from the molecules dynamic simulation at the temperature of 300 K.



Figures S2. Band edges and total energy as a function of uniaxial strain. (a), (b) and (c) are the linear fitting of band edges and (d), (e) and (f) are the quadratic fitting of total energy for α-AsSb, γ-AsSb and ε-AsSb respectively.