Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Electronic structures and optical properties of arsenene and antimonene under strain and electric field

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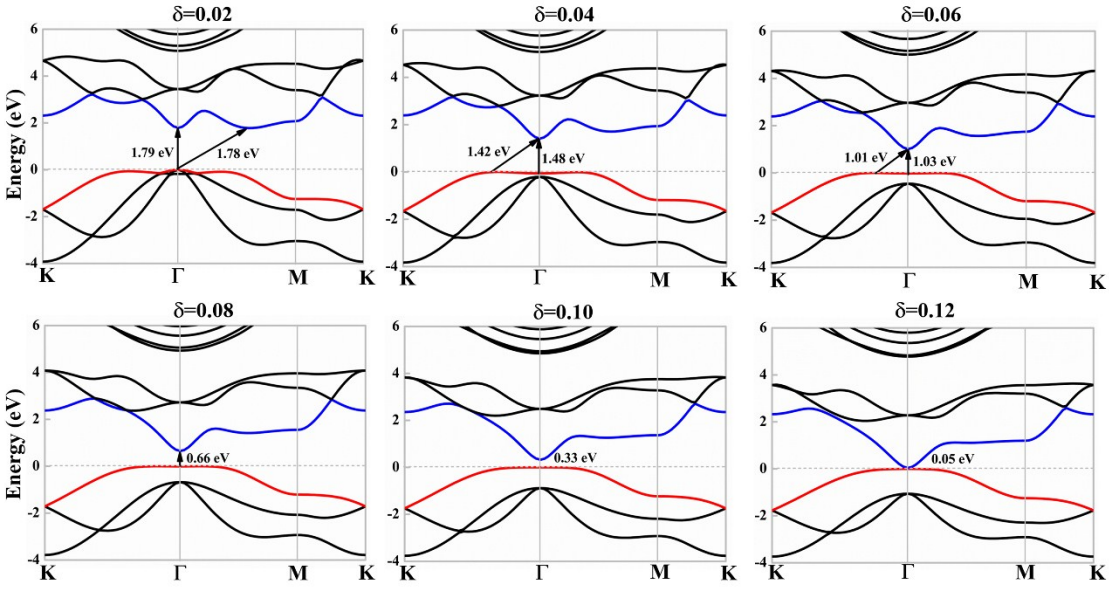

Figure S1. The band structures of β-As under the different tensile strain. The blue and red solid lines show two band edges.

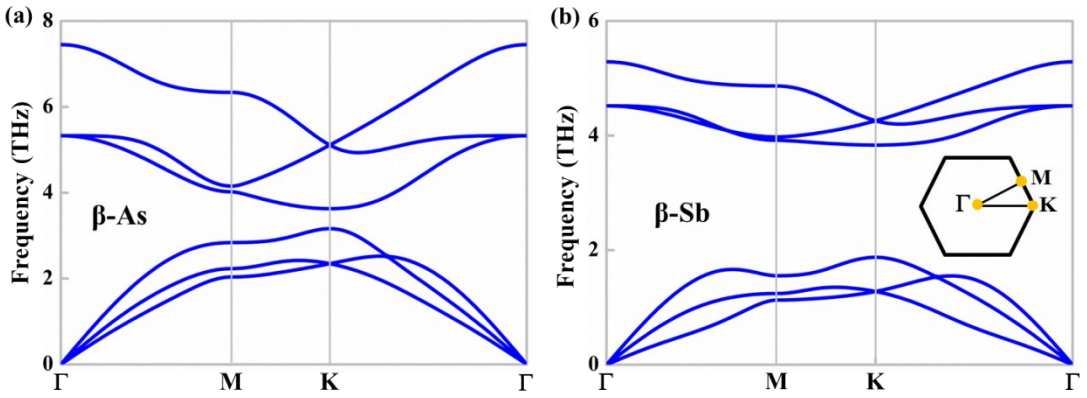

Figure S2. Phonon dispersion under biaxial tensile strain of 12%: (a) β-As, (b) β-Sb.

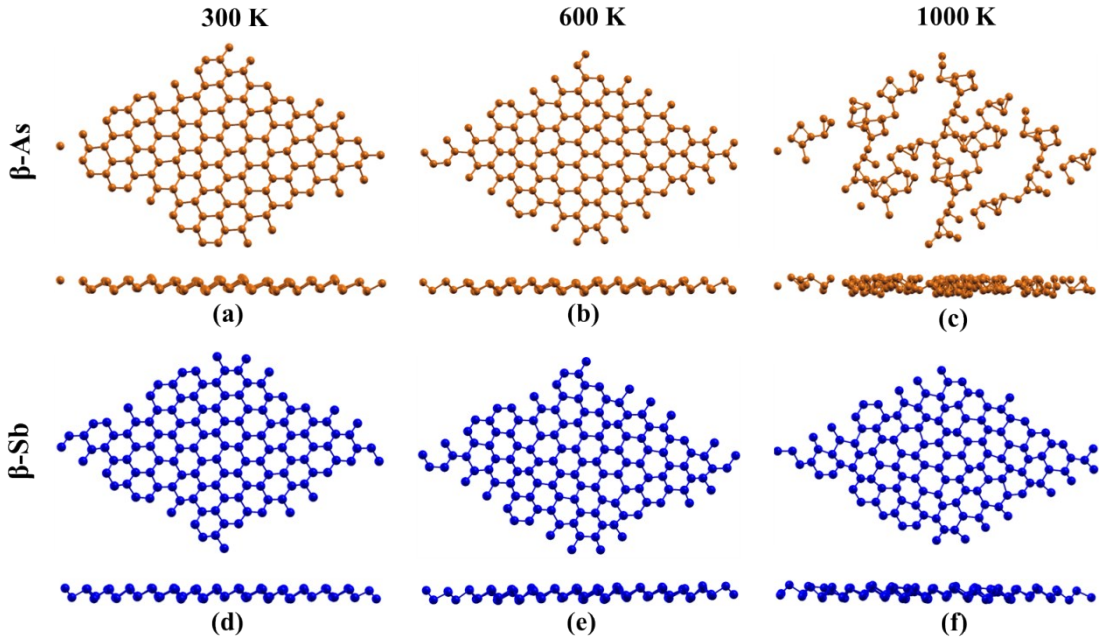

Figure S3. Snapshots of atomic structures of β-As (a-c) and β-Sb (d-f) obtained by molecular dynamics calculations at T= 300, 600 and 1000 K, respectively.

Table S1. Structural parameters and energy bandgaps of the β-As and β-Sb: Lattice a (Å), bond length l (Å), bond angle θ (^{0}), and buckling height Δ (Å); $E_{g\text{-}PBE}$ (eV) and $E_{g\text{-}G_0W_0}$ (eV) at the DFT-PBE and G_0W_0 levels, respectively. The unit of the electric field is V/Å. "i" and "d" show the indirect and direct bandgap, respectively.

Name	Field	a	l	Δ	θ	$E_{g\text{-}PBE}$	$E_{g\text{-}G_0W_0}$
β-As	0.00	3.635	2.5216	1.4053	91.951	1.61 (i)	2.70 (i)
	0.60	3.641	2.5221	1.4064	91.925	0.82 (d)	1.11 (d)
	0.70	3.644	2.5243	1.4103	91.822	0.00	0.00
β-Sb	0.00	3.982	2.8047	1.6110	90.295	1.10 (i)	2.25 (i)
	0.60	3.986	2.8061	1.6133	90.238	0.43 (d)	0.53 (d)
	0.63	3.991	2.8062	1.6135	90.234	0.00	0.00

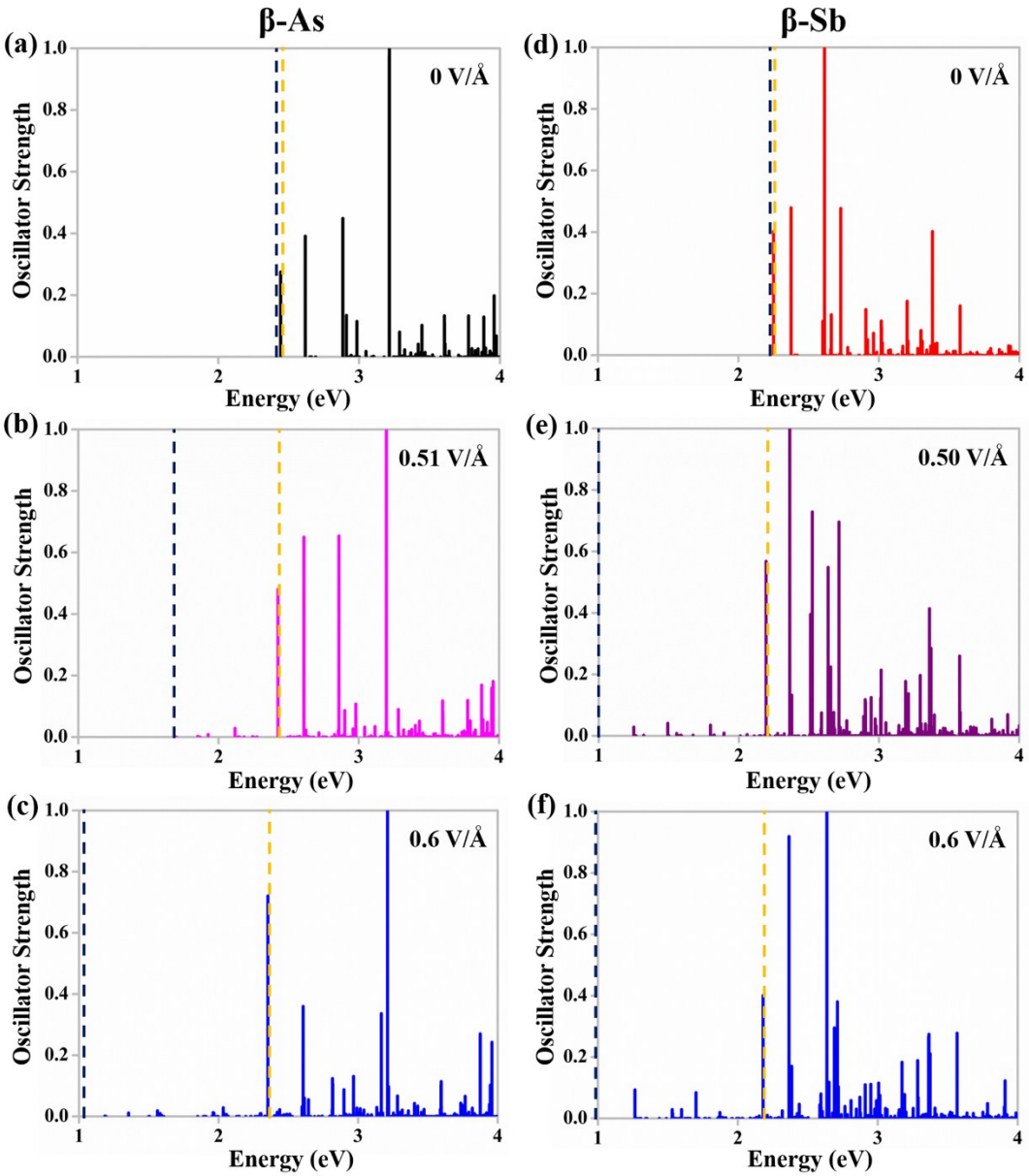

Figure S4. Oscillator strengths of the excited states for incident light polarization parallel to the surface (along the lattice vector ***a*** direction) under externally electric field: (a)-(c) β-As and (d)-(f) β-Sb. Two dot lines show the positions of the first dark state (black) and first bright excited state (orange), respectively.