Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

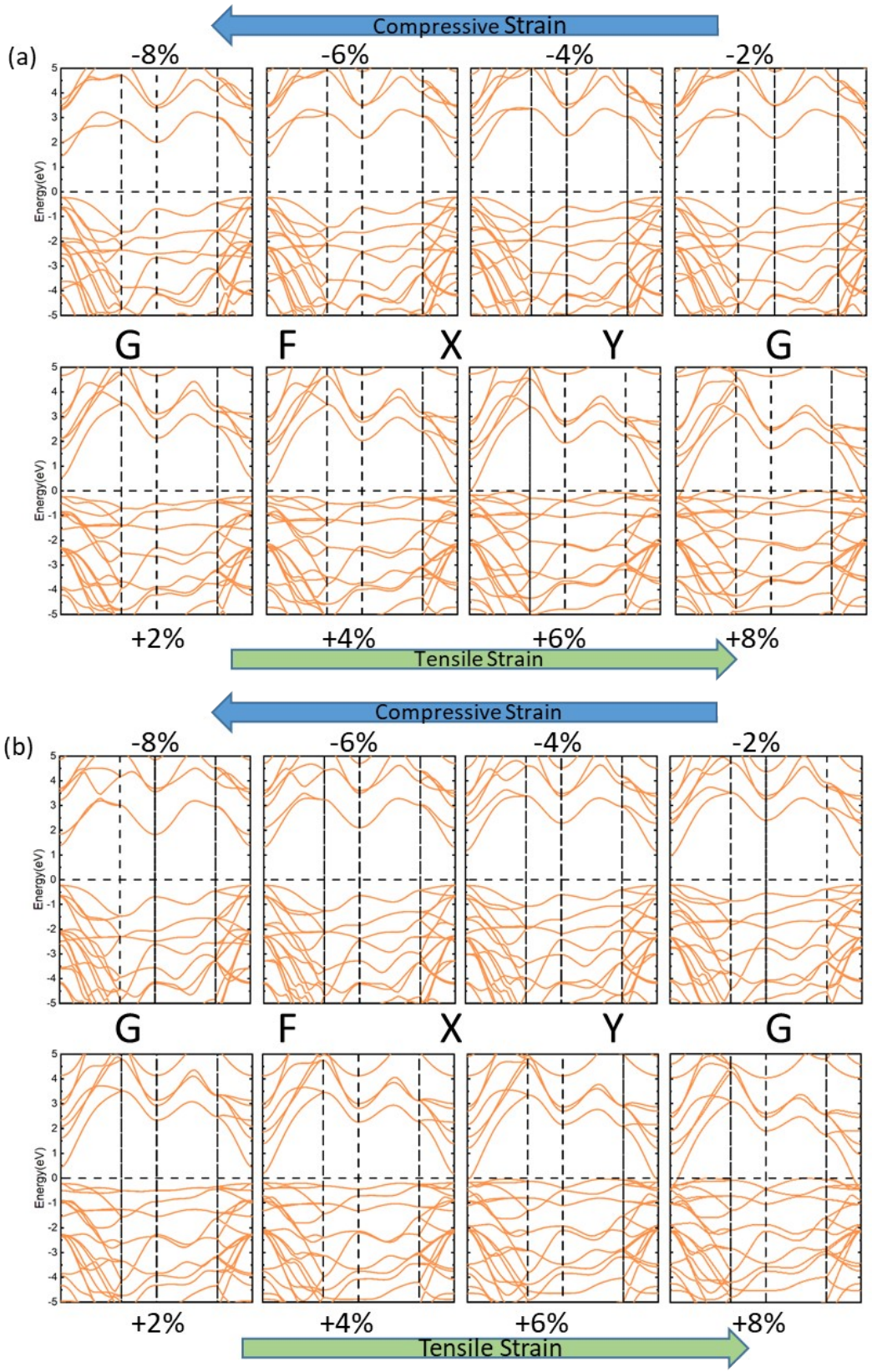

Figure S1. Band structure variation under biaxial strain for **(a)** H and **(b)** H′ phase $SnGe_2N_4$.

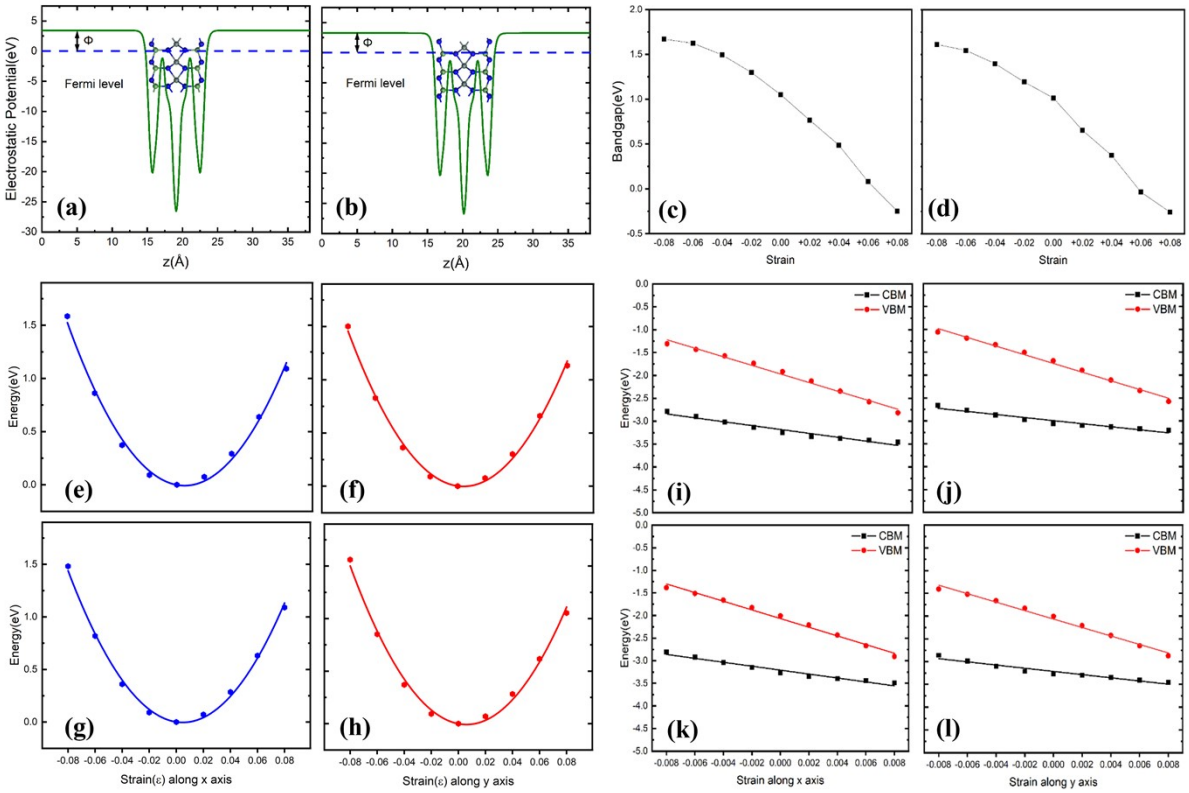

Figure S2. (a, b) The work function along the z-axis, **(c, d)** bandgap variation with biaxial strain, **(e-h)** Energy strain curve and **(i-l)** variation of CBM and VBM with x and y uniaxial strains for H and H′ phase $SnGe_2N_4$, respectively.

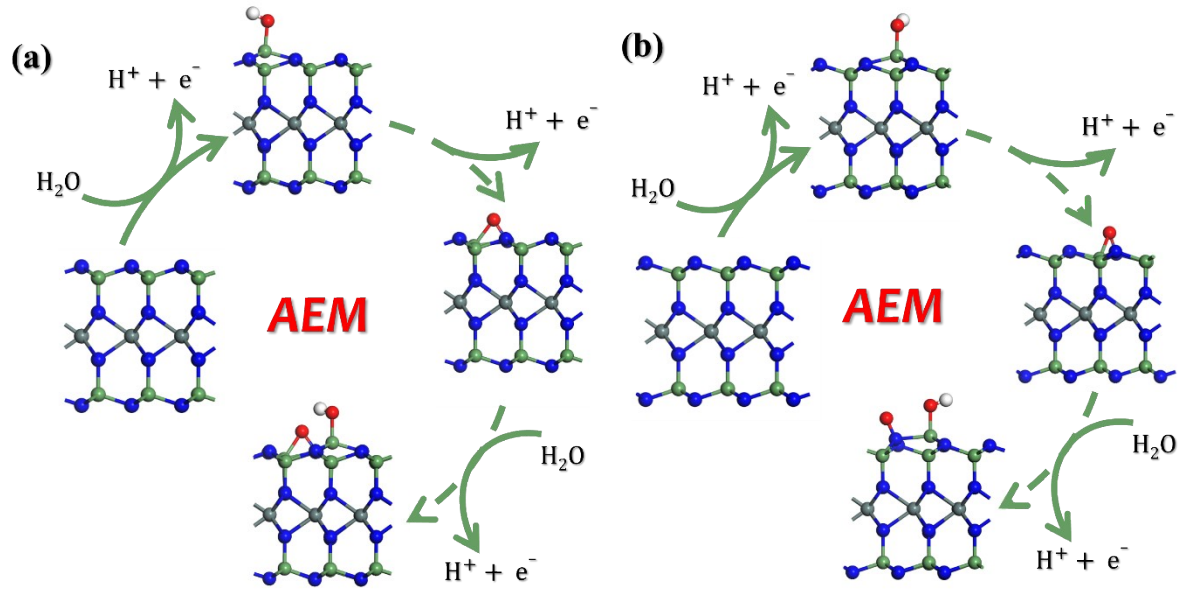

Figure S3. The deviation of OER from conventional AEM pathway for (a) H-$SnGe_2N_4$ and (b) H′-$SnGe_2N_4$.

Table S1. Optimized lattice parameters a in Å, band gap E_g in eV, bond lengths d_{Sn-N} and d_{Ge-N} in Angstrom (Å), elastic constants C_{11}, C_{12}, C_{22} and C_{66} in Nm^{-1}, Young's modulus Y_{2D} in Nm^{-1} and Poisson's ratio ν for H and H′ $SnGe_2N_4$.

	a	E_g (eV)	d_{Sn-N} (Å)	d_{Ge-N} (Å)	C_{11} (Nm^{-1})	C_{12} (Nm^{-1})	C_{22} (Nm^{-1})	C_{66} (Nm^{-1})	Y_{2D} (Nm^{-1})	ν
H	3.097879	1.0524	2.14882	1.88698	399.479	120.451	393.067	139.465	349.9951	0.306439
H′	3.099028	1.0151	2.14975	1.88730	380.367	116.046	386.904	135.974	386.904	0.299935

Table S2. Bader charge analysis for H and H′ phase $SnGe_2N_4$.

	Bader net charge (e)		
System	**Sn**	**Ge**	**N**
H-$SnGe_2N_4$	-1.9402	-1.9471	1.4779
H′-$SnGe_2N_4$	-1.9318	-1.9855	1.4755