

Prediction of hydrogenated group IV-V hexagonal binary monolayers

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TABLE S1. Structural parameters for the pure X_2Y binary compound monolayers, including lattice constants (a), bond lengths (R_{XX} & R_{XY}), and buckling heights (Δ).

	a (Å)	R_{XX} (Å)	R_{XY} (Å)	Δ (Å)
Si ₂ P	6.33	2.31	2.26	0.86
Si ₂ As	6.51	2.31	2.38	1
Si ₂ Sb	6.85	2.32	2.59	1.13
Si ₂ Bi	6.99	2.32	2.68	1.21
Ge ₂ P	6.59	2.48	2.36	0.89
Ge ₂ As	6.77	2.48	2.47	1.02
Ge ₂ Sb	7.09	2.48	2.67	1.17
Ge ₂ Bi	7.23	2.47	2.75	1.24

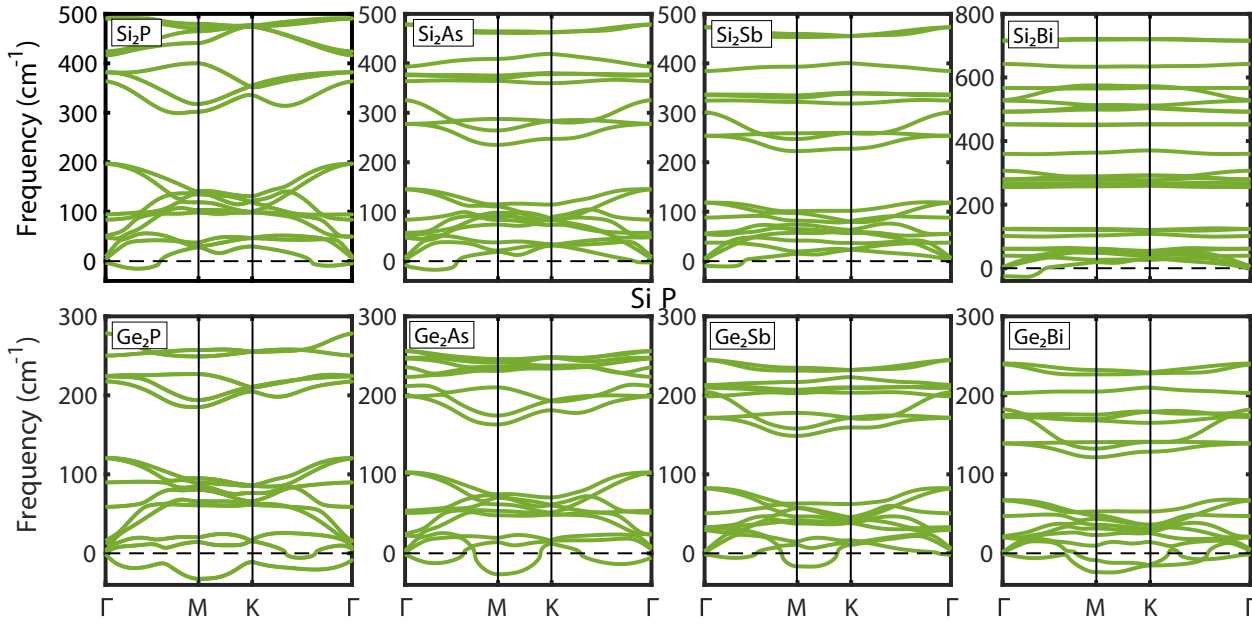


FIG. S1. Phonon dispersion calculations of the pure X_2Y binary compound monolayers. All the structures are dynamically unstable.

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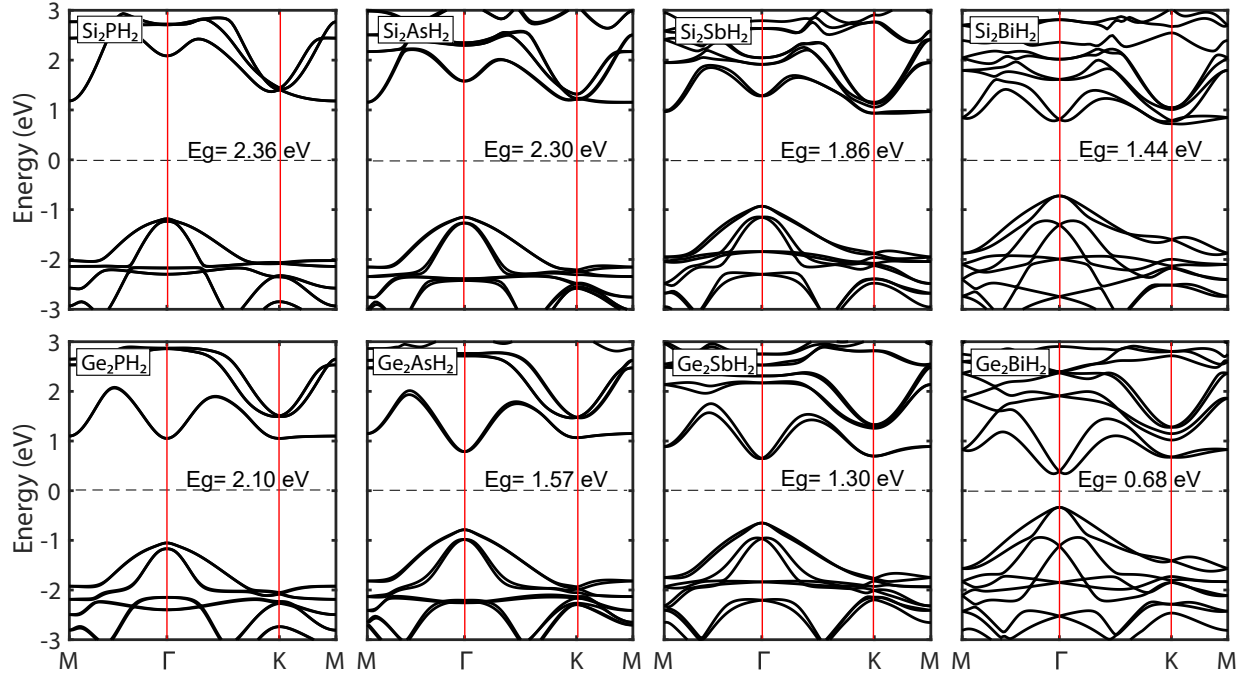


FIG. S2. Energy band structures of the X_2YH_2 binary compound monolayers along the main high symmetry k-points in the presence of spin-orbit coupling (SOC) together with the band gap amounts. The Fermi level has been set to zero.

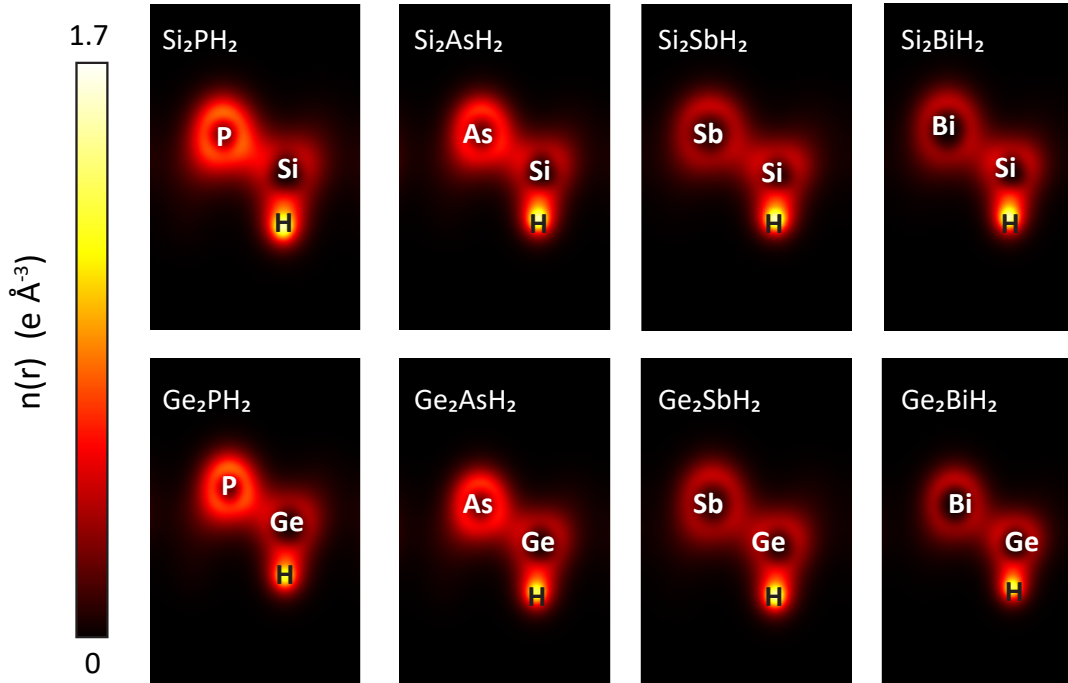


FIG. S3. Electron density of the X_2YH_2 binary compound monolayers at GGA level.

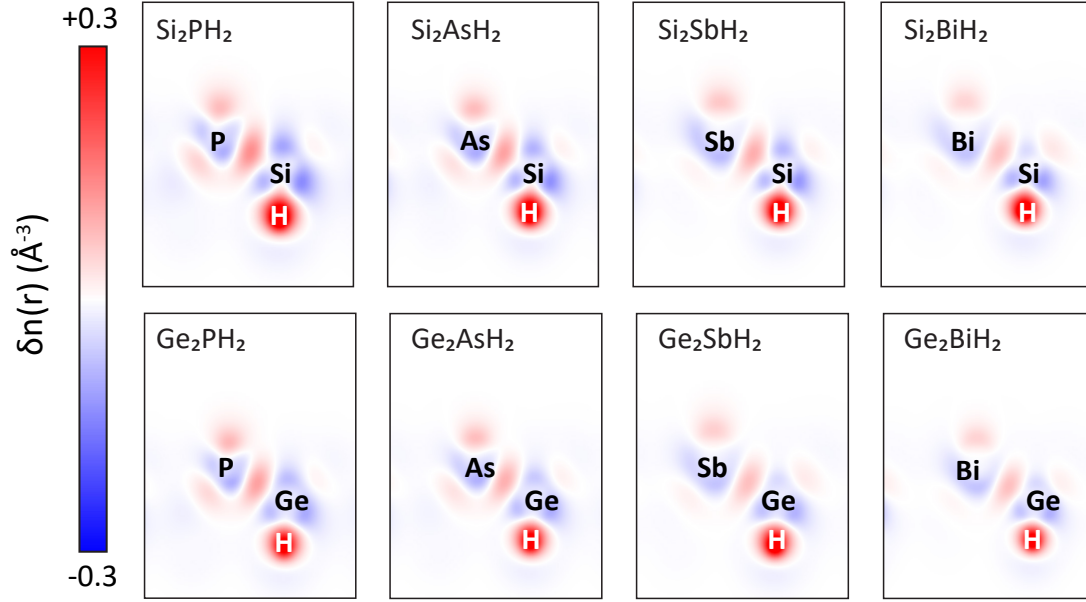


FIG. S4. Electron difference density of the X_2YH_2 binary compound monolayers at GGA level.

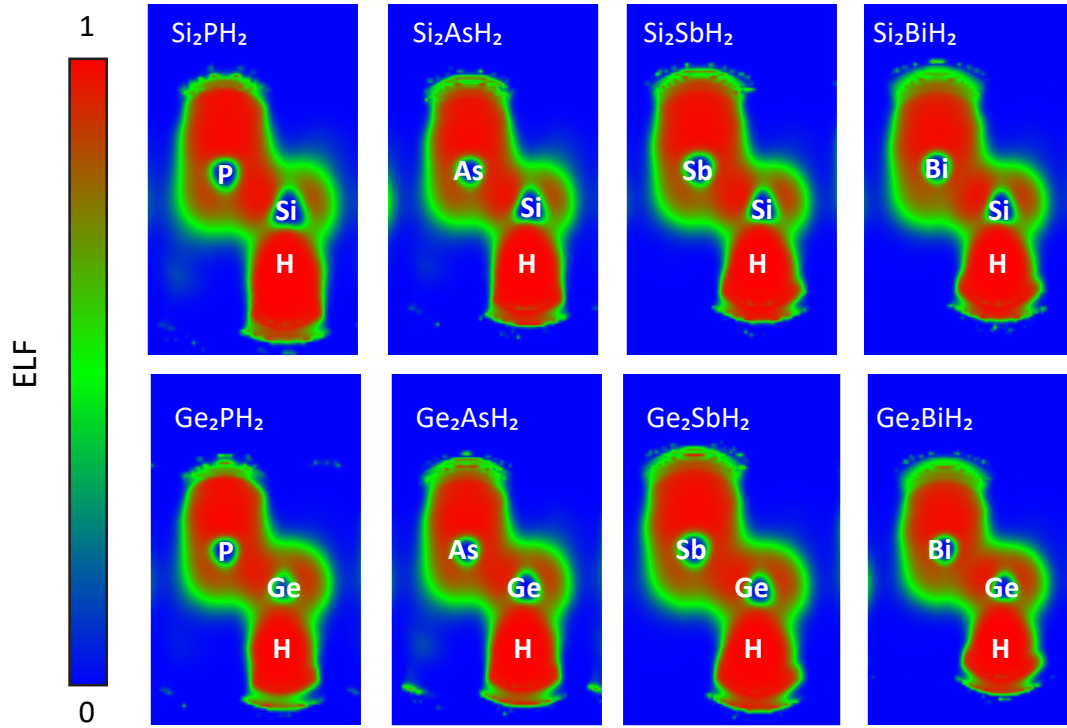


FIG. S5. The electron localization function (ELF) of the X_2YH_2 binary compound monolayers at GGA level.