

Supporting information for

Prediction of topological phase transition in X2-SiGe monolayers

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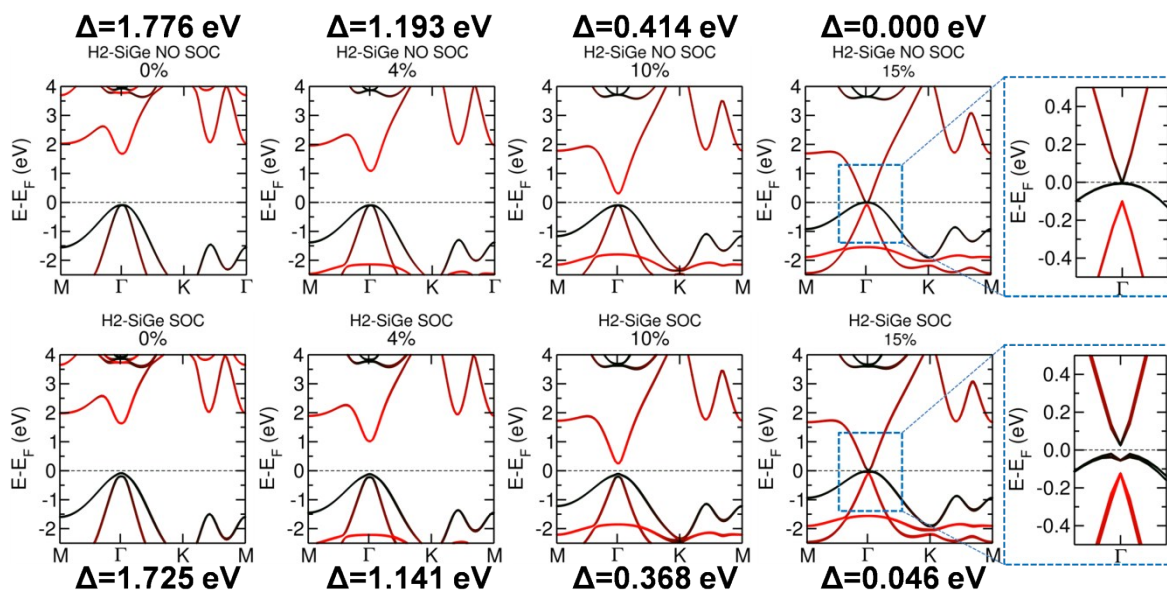


Figure S1. Evolution of the band structure of a H2-SiGe monolayer under strain. The band structures are calculated without (upper) and with (lower) SOC. The zoomed-in of the closest bands to the Fermi level for the 15%-strained H2-SiGe monolayer are shown right-most plots. Δ stands for the band gap at each percentage of strain. The color gradient

indicates the contribution of the s , p_x , and p_y orbitals to each of the bands along the k-path – red for s , and dark blue for p_x , and p_y .

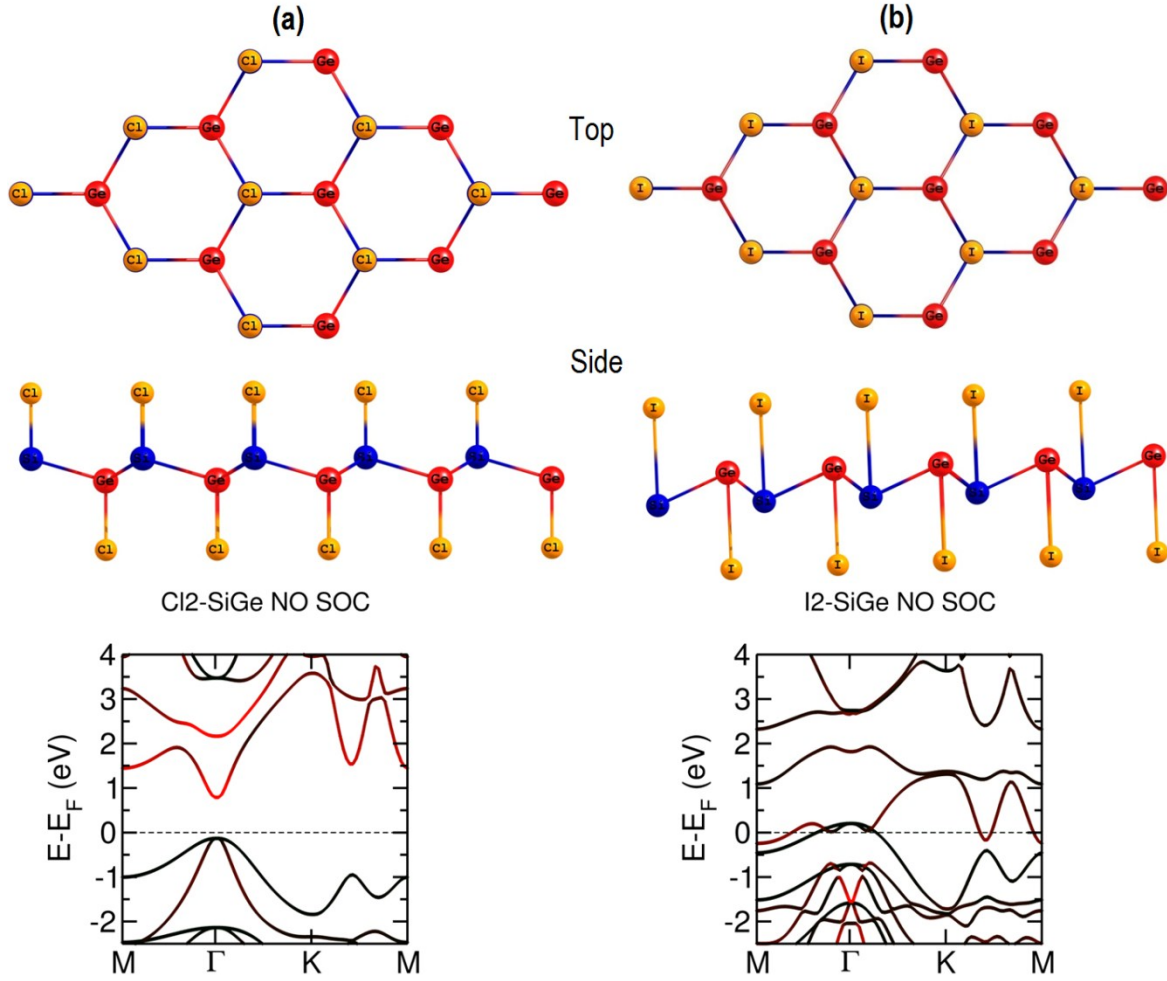


Figure S2. Top and side views of the optimized (a) Cl2-SiGe and (b) I2-SiGe structures with their corresponding band structure. The calculated bond distances for I2-SiGe are $d_{\text{Si-I}} = 3.196 \text{ \AA}$, $d_{\text{Ge-I}} = 3.160 \text{ \AA}$, $d_{\text{Si-Ge}} = 2.522 \text{ \AA}$, while for Cl2-SiGe are $d_{\text{Si-Cl}} = 2.080 \text{ \AA}$, $d_{\text{Ge-Cl}} = 2.188 \text{ \AA}$, $d_{\text{Si-Ge}} = 2.451 \text{ \AA}$. The color gradient in the plots indicates the contribution of the s , p_x , and p_y orbitals to each of the bands along the k-path – red for s , and dark blue for p_x , and p_y .

