Supplementary Information

Prediction of Band Inversion in Janus In_2XYZ (X, Y, and Z= S, Se, Te) monolayers

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In this work, the electronic and spin characteristics of Janus In_2X_2Y and In_2XYZ (X, Y, and Z= S, Se, Te) monolayers are explored. The two sides of these Janus compounds have distinct vacuum levels due to their vertical asymmetry, which causes different work functions. An emerging dipole moment alters the band alignments on both surfaces of Janus In_2X_2Y structures due to electronegativity differences between various chalcogen atoms on each surface. The band structures of these monolayers with and without spin-orbit coupling (SOC) are compared. The SOC consideration opens a finite bandgap in In_2STeS, In_2SSTe, $In_2SeTeSe$, and $In_2SeTeTe$ monolayers while demonstrating a metallic behavior without SOC. The band inversion is indicated in these monolayers using projected band structures. In addition, In_2SSeTe and In_2SeTeS monolayers exhibit the band inversion, and In_2SeTeS has the highest topological bandgap as 111 meV.

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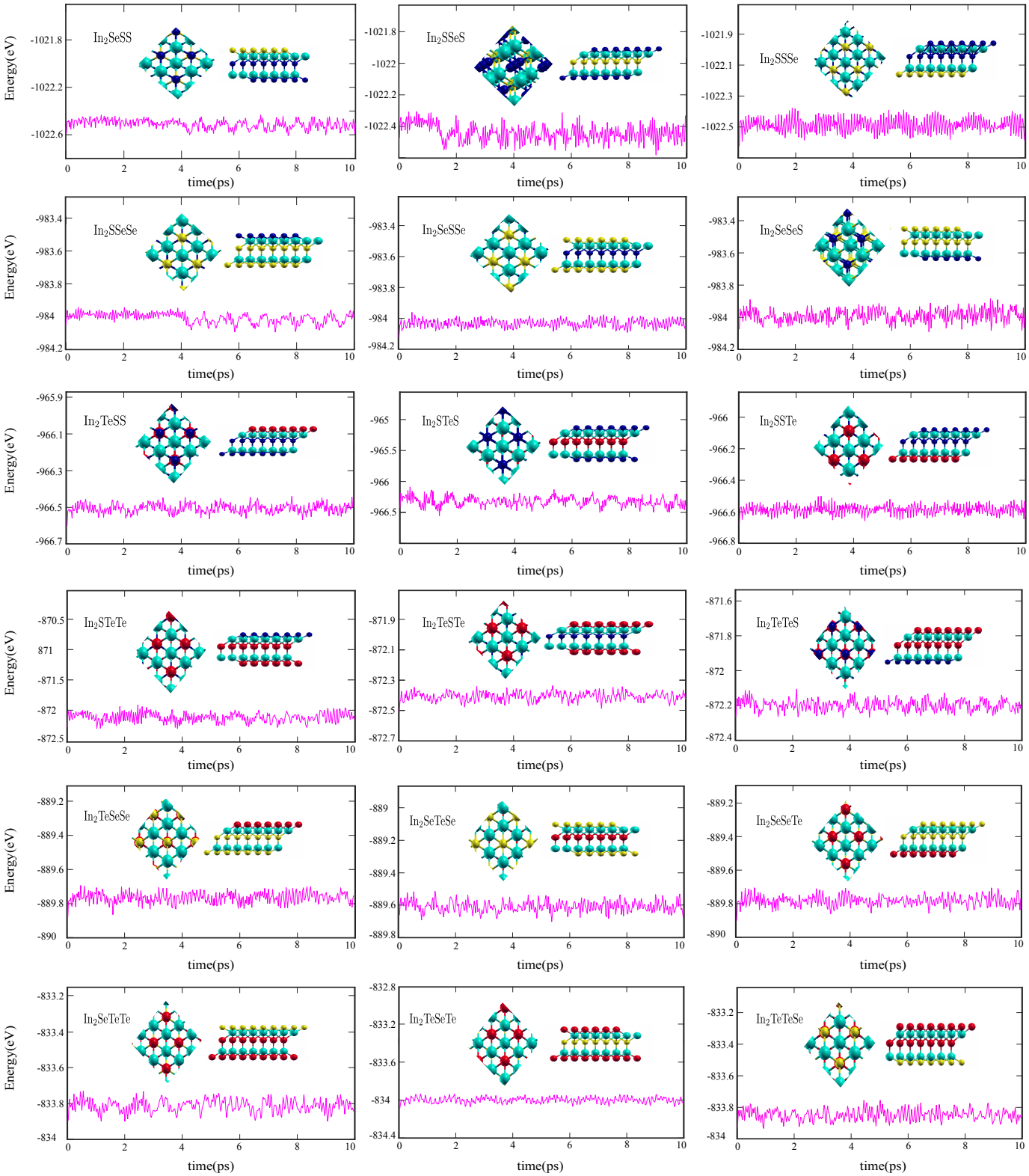

Figure 1 Ab initio molecular dynamics (AIMD) for the In_2X_2Y monolayers at room temperature. The top and side views of the structures after 10 ps of simulation are indicated as inset.

Fig. 1 illustrates ab inito molecular dynamics (AIMD) for the In_2X_2Y monolayers at room temperature. Fig. 1 displays the top and side views of the structures as insets after 10 ps of simulation. The structures could maintain their integrity at 300 K with a very steady energy and temperature profile, demonstrating the thermal stability of the In_2X_2Y monolayers, according to the analysis of the AIMD trajectories.

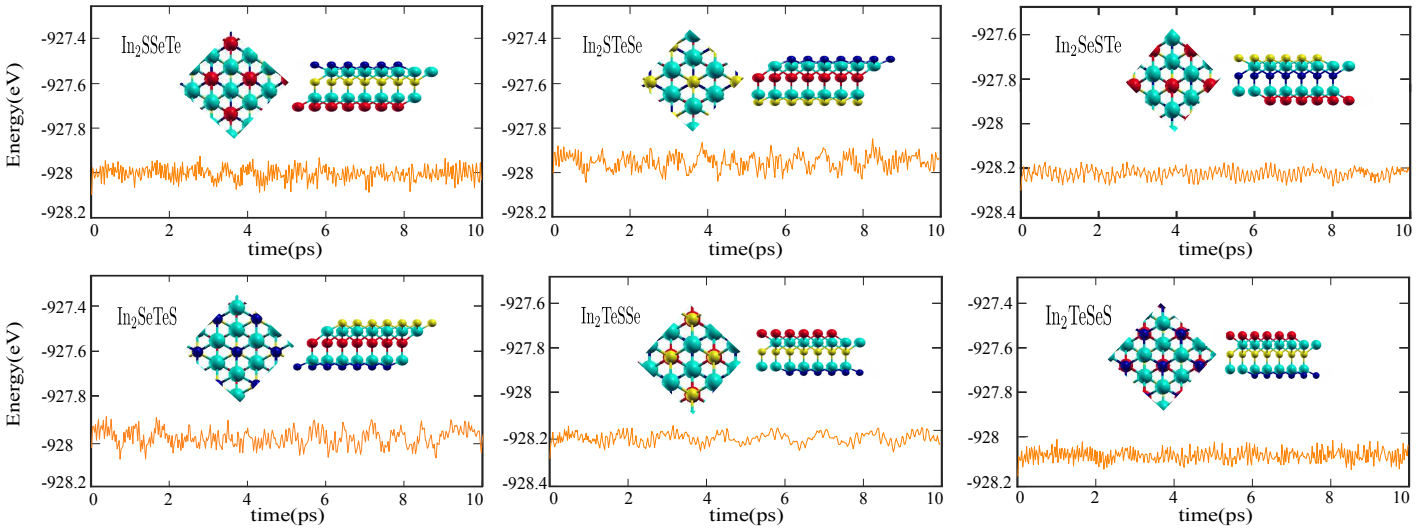

Figure 2 AIMD simulations of the total energy profiles of In_2XYZ structures at 300K. Top and side views of the corresponding atomic structures after an AIMD simulation period of 10 ps are shown. The In, S, Se and Te atoms are shown by light blue, dark blue, yellow, and red colors, respectively.

An AIMD simulation then examines the thermal stability of In_2XYZ structures. During the AIMD simulation time of 10 ps with a temperature of 300 K, the predicted total energy of the In_2XYZ monolayers is shown in Fig. 2. Also, Fig. 2 displays top and side views of the matching atomic structures before and after the AIMD simulation. At 300 K, there is minimal variance in the total energy, less than 0.1 eV.