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Supplementary Material

The Thermal Stability of Janus Monolayers SnXY (X, Y = O, S, Se): Ab-Initio Molecular Dynamics and Beyond

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1. The phonon dispersion relations of Janus monolayers SnXY (X, Y = O, S, Se)

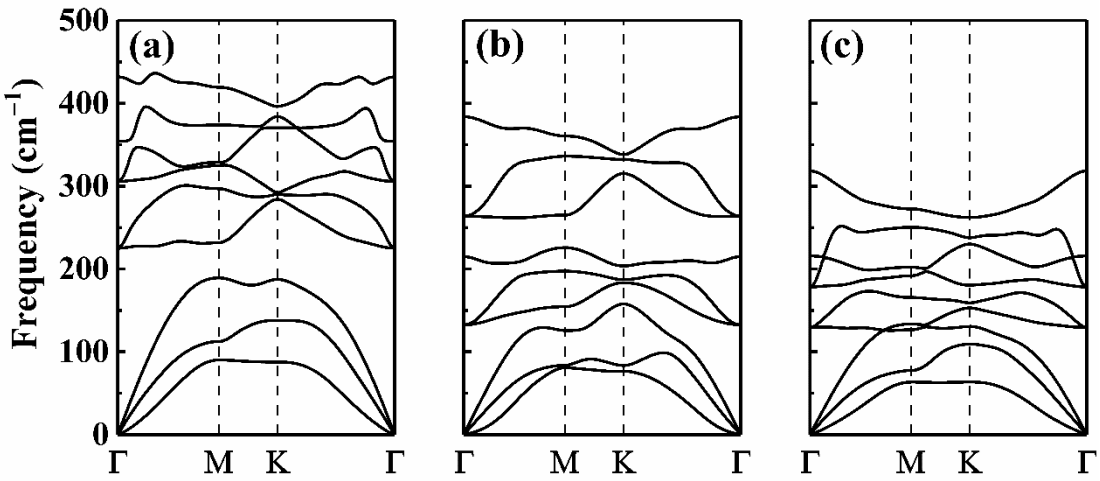

Figure S1. The phonon dispersion relations of Janus monolayers (**a**) SnOS, (**b**) SnOSe and (**c**) SnSSe.

2. The *ab-initio* molecular dynamics (AIMD) simulations for the Janus monolayers SnXY (X, Y = O, S, Se)

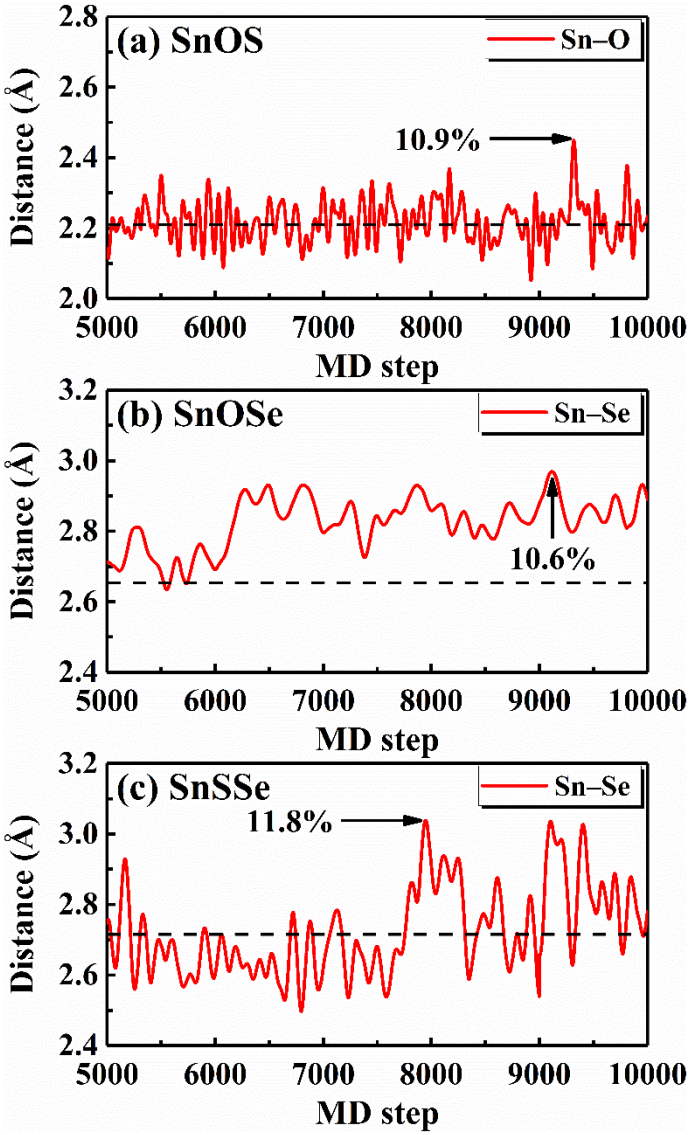

Figure S2. The AIMD results of the bond distances for the Janus monolayers (**a**) SnOS at 525 K, (**b**) SnOSe at 100 K, and (**c**) SnSSe at 825 K. For each case, only that with larger fluctuation around the equilibrium length is shown.

3. The AIMD simulations for the TMD monolayers SnX_2 (X = O, S, Se)

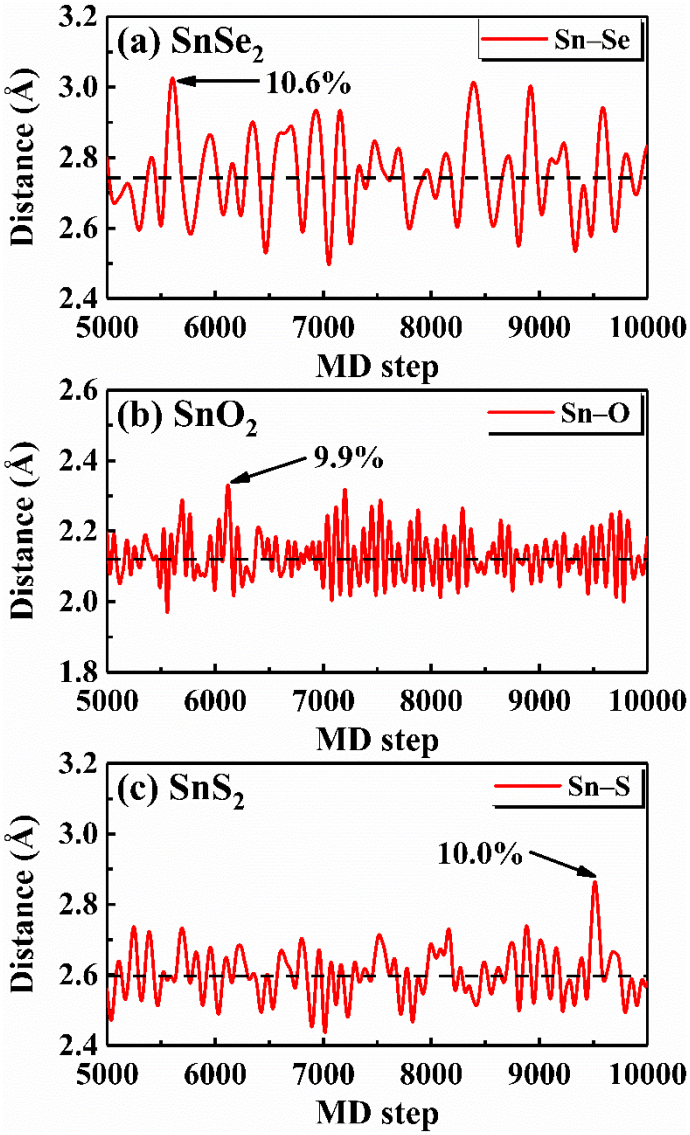

Figure S3. The AIMD results of the bond distances for the monolayers (**a**) $SnSe_2$ at 437 K, (**b**) SnO_2 at 500 K, and (**c**) SnS_2 at 675 K, where the maximum fluctuations around the equilibrium lengths are shown.