Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Low thermal conductivity and high performance anisotropic thermoelectric properties of XSe (X=Cu, Ag, Au) monolayers

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The Electron Localization Function (ELF)

To explain the charge transfer and the bond nature between the square-planar X^{IV} atom, the linear X^{II} atom with Se atoms in the 2D systems, we calculated the electron localization function. Results show that the electrons are mainly localized around the Se atoms, suggesting that the electrons transfer from X to the Se atom. For the linear X^{II} atom, the localized electrons are far away from the X-Se bond at the outer part of Se atoms. These results indicate that the lone-pair electrons (LPEs) and the partial-ionic band exist in our studied systems. For the square-planar X^{IV} atom, the localized electrons aggregating long the X-Se band and close to the Se atoms indicates a polarized covalent bonding nature.

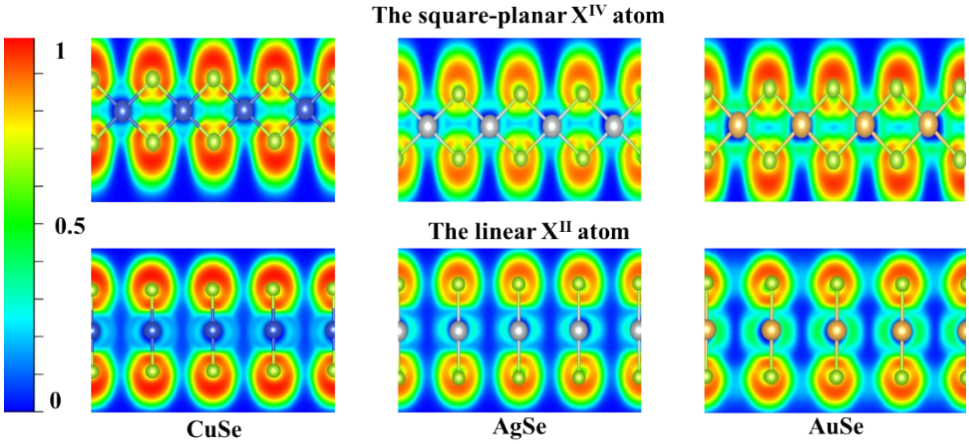

Figure S1. The electron localization function (ELF) for X^{IV}-Se and X^{II}-Se of XSe monolayers

The Thermal Stability

The thermodynamic stability of the 2D system is of great importance. We run the ab-initio molecular dynamics (AIMD) simulations at 900 K for these monolayers. Results show that these monolayers can be maintained up to 10 ps at 900 K, suggesting they are stable at high temperature.

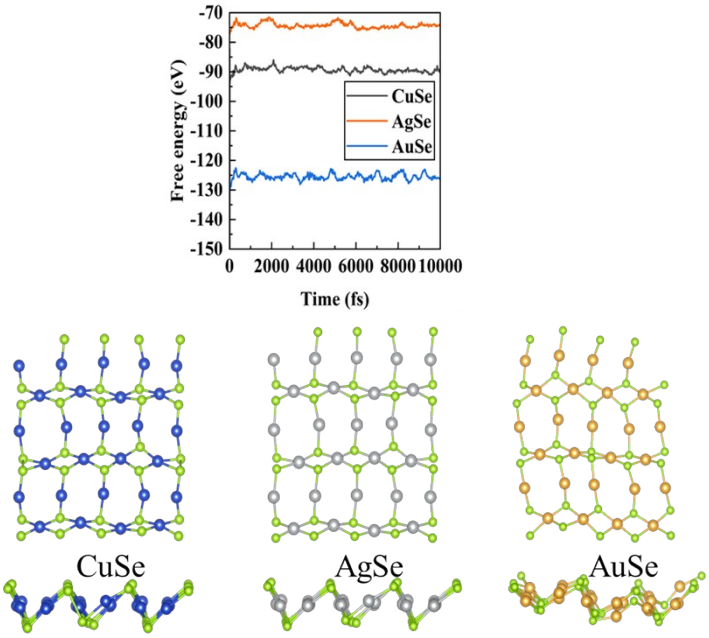

Figure S2. Free energy fluctuations with respect to time and equilibrium structures of these monolayers by AIMD simulations at 900 K.