Supplementary Materials: First Principles Study of Gas Molecules Adsorption on Monolayered β-SnSe

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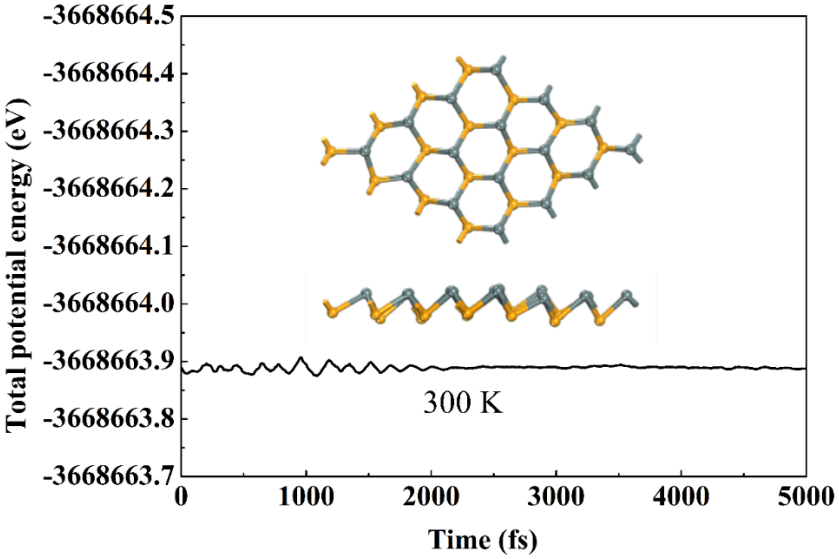

Figure S1. Total potential energy of pristine monolayer SnSe at 300 K within 5 ps during the first-principles molecular dynamics (MD) simulation.

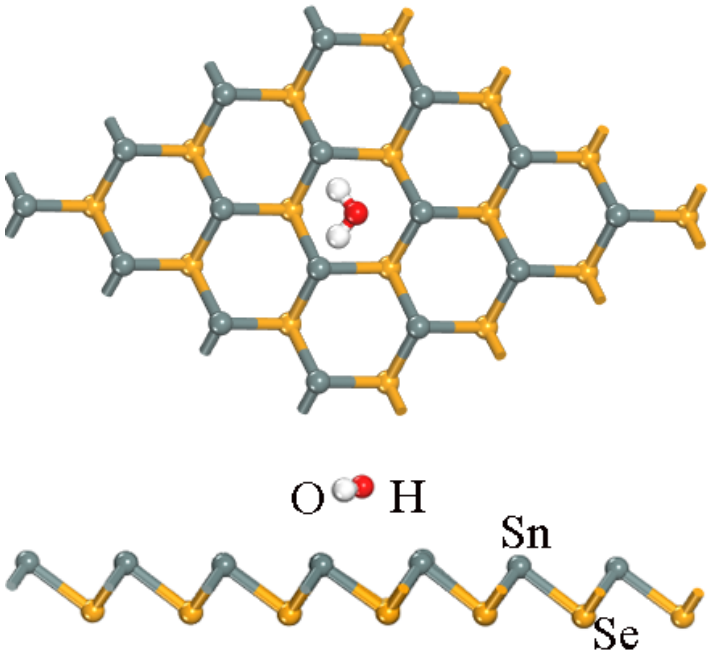

Figure S2. The most stable site of structural optimizations for H_2O on β-SnSe layer is presented.

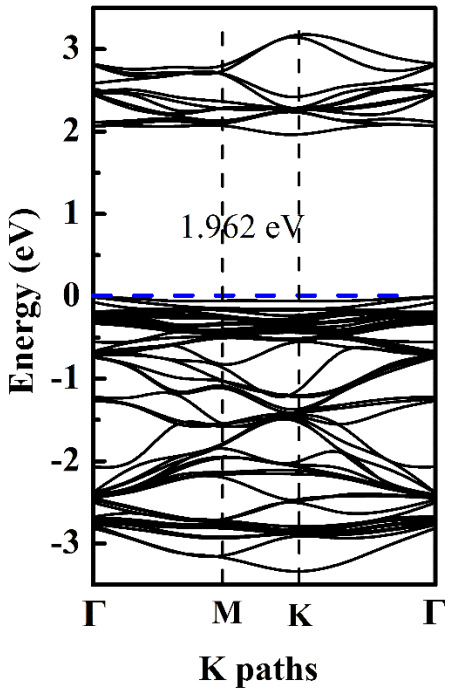

Figure S3. Band structure of the monolayered β-SnSe with the H_2O molecules.

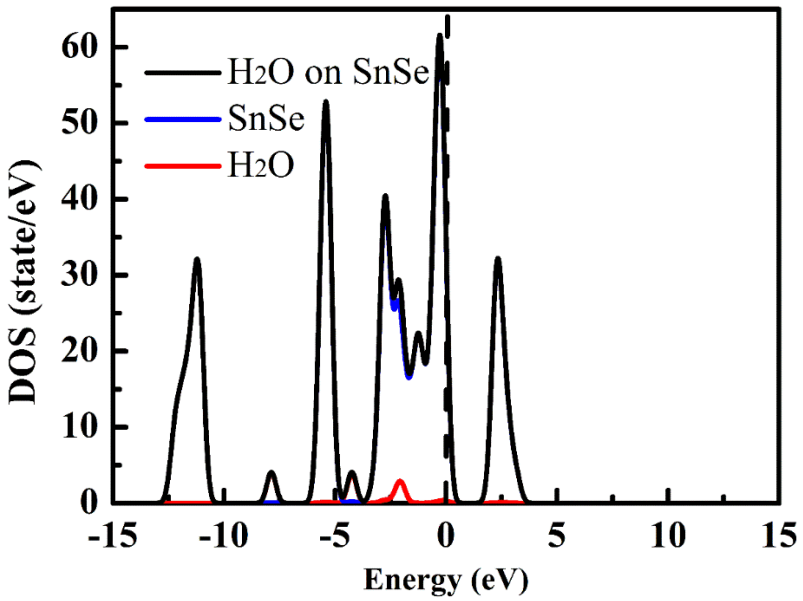

Figure S4. Total DOSs of the H_2O on SnSe (black curve), the projected DOS of SnSe (red curve), and the adsorbate molecules (blue curve) for H_2O on SnSe monolayer. The E_f is set to zero, as illustrated by black dotted line.

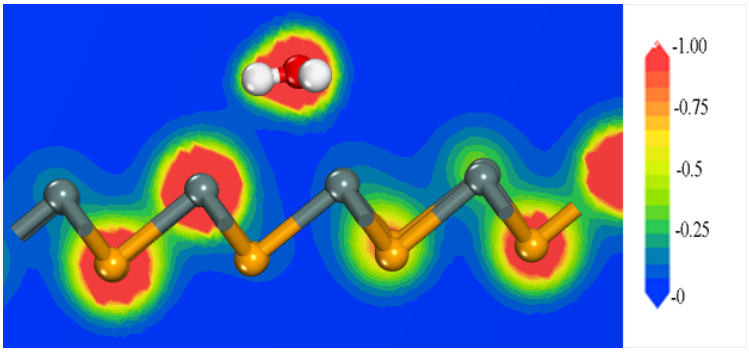

Figure S5. The slice of charge densities for the β-SnSe monolayer with the H_2O molecule. The value of electron densities ranges between 0 and 1.00 e/Å^3.