Supporting Information

Charging assisted structural phase transitions in monolayer InSe

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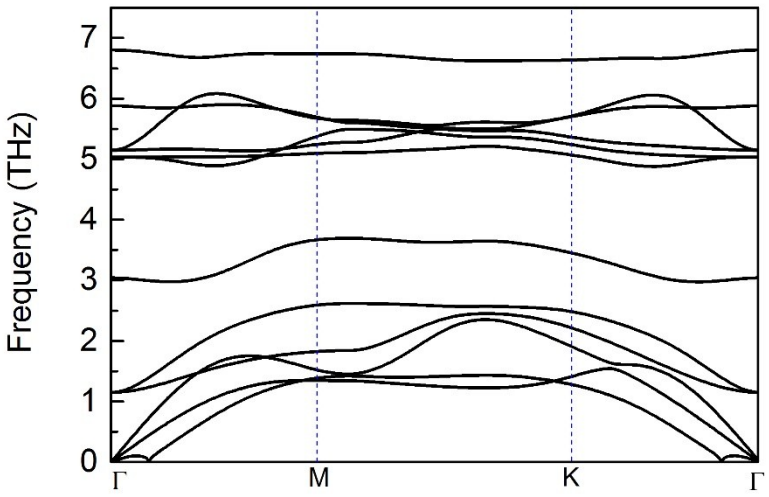

Figure S1. Calculated phonon frequency of β-InSe monolayer using a 5×5 supercell. No imaginary frequency is observed, confirming the dynamical stability of the experimentally synthesized structure.

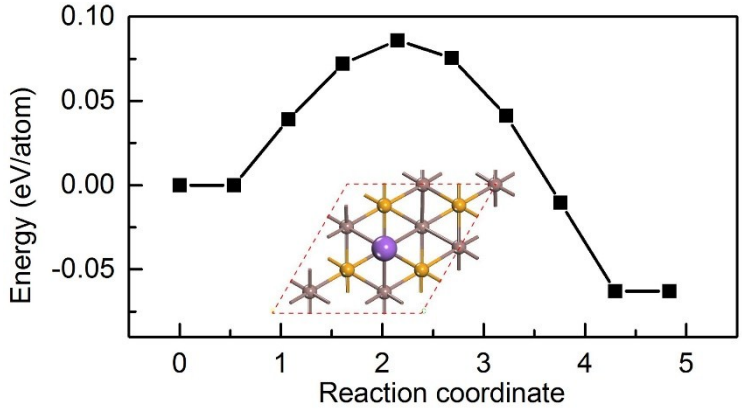

Figure S2. Calculated energy barrier (0.09 eV/atom) for the γ-β phase transition with ¼ sodium adsorption. The inset depicts the relaxed structure of γ-InSe with ¼ sodium adsorption.

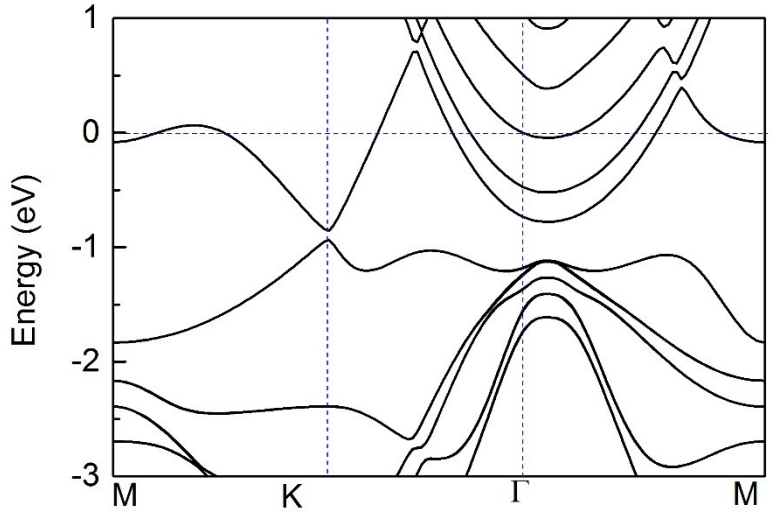

Figure S3. Calculated (with SOC included) electronic band structure of γ-InSe monolayer with two electron injection into the unit cell.

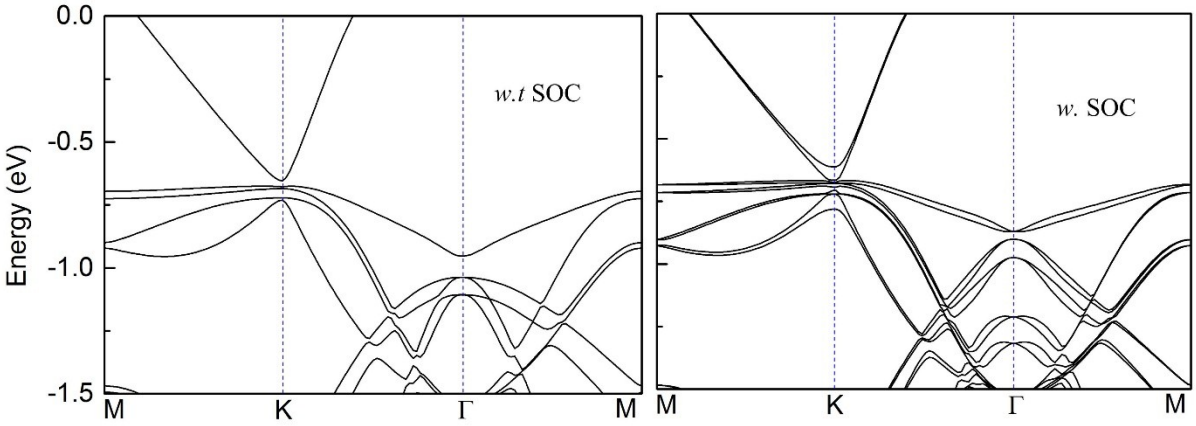

Figure S4. Calculated electronic band structures of Na decorated γ-InSe monolayer without and with SOC.

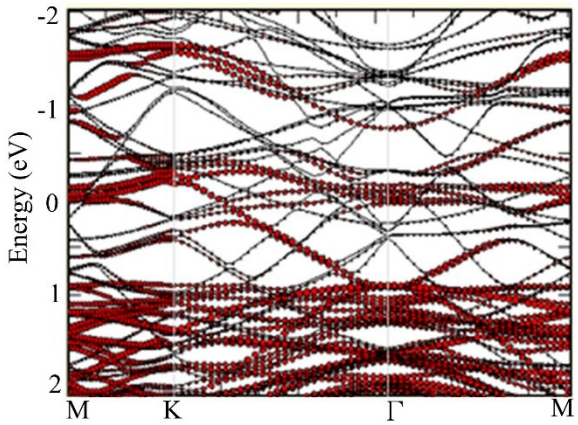

Figure S5. Calculated electronic band structure of γ-InSe monolayer on the Ag (111) surface; the states from InSe are represented by the red dotted lines.

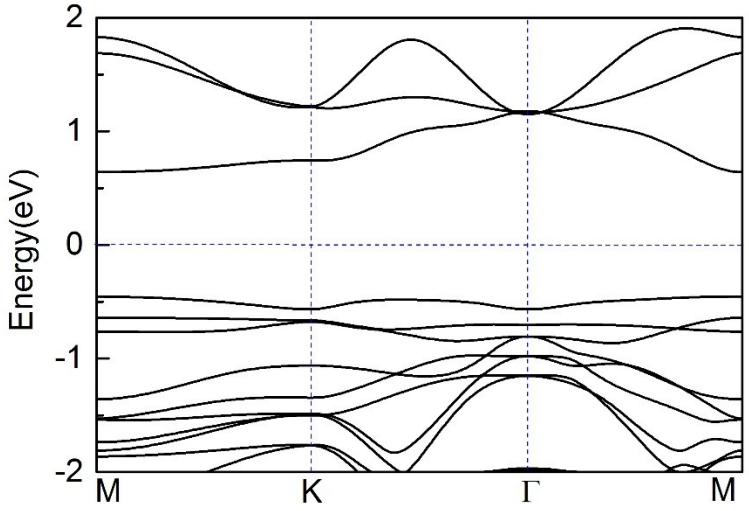

Figure S6. Calculated electronic band structure of the distorted γ-InSe monolayer.

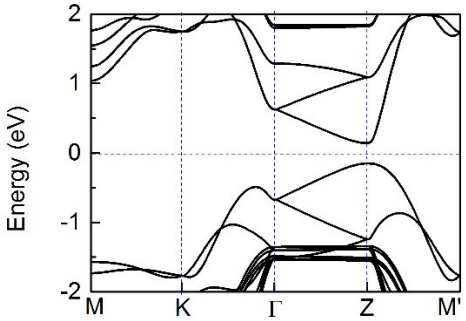

Figure S7. Calculated electronic band structure of the bulk β-InSe.

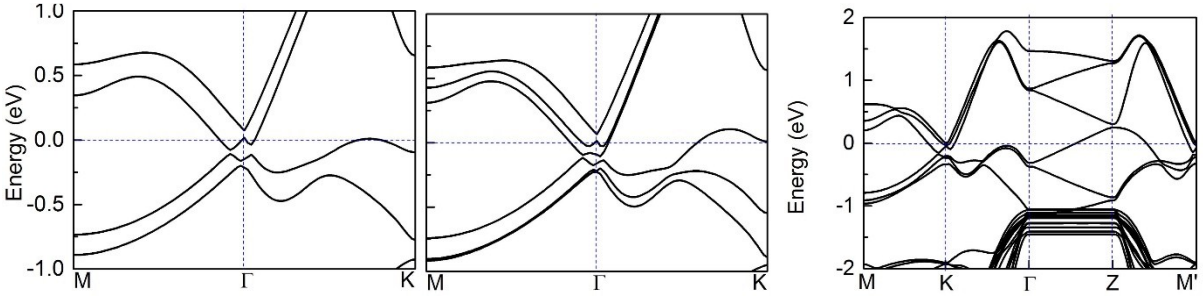

Figure S8. Electronic band structures of the bilayer (left), trilayer (middle) and bulk (right) γ-InSe.