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

Supplementary Materials to

Tuning the Electronic and Magnetic Properties of InSe Nanosheets by Transition Metal Doping

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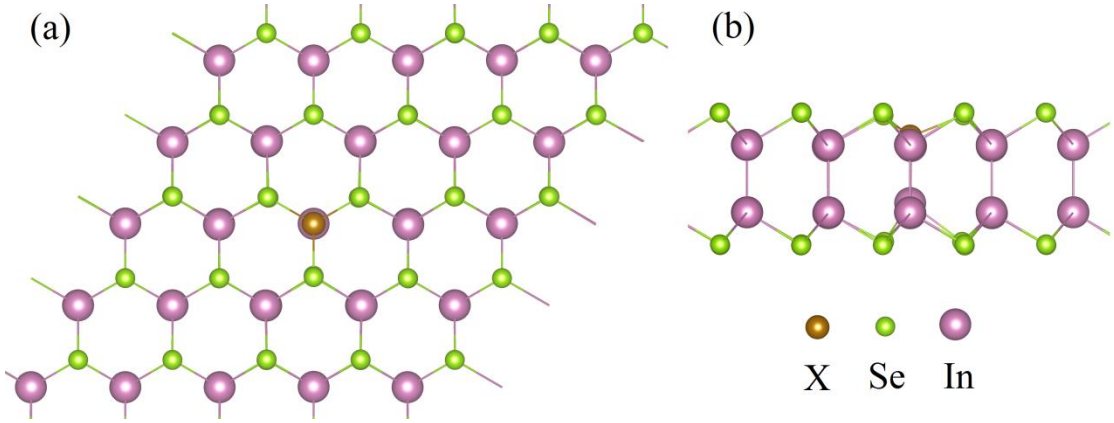

Figure S1. (a) Top view and (b) side view of InSe supercell.

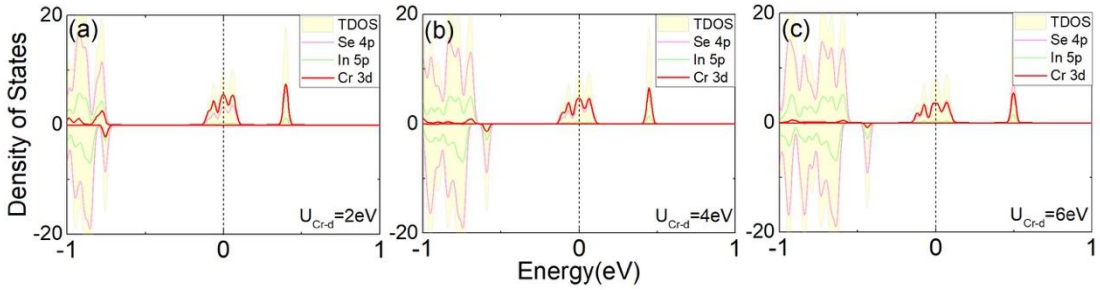

Figure S2. DOS of Cr-InSe with UCr-d = (a) 2eV, (b) 4eV, and (c) 6eV.

In this study, a GGA+U approach is also employed to test whether the standard DFT can correctly describe the TM-doped systems. We choose different U values and

calculate the electronic and magnetic properties of Cr-doped InSe monolayer. As shown in **Figure S2**, the DOS of Cr-doped InSe monolayers are almost independent of the U values, especially around the fermi energy. All of the studied monolayers with different U values show half-metallic behaviors, which may be ascribed to the low concentration of the TM elements in our systems.

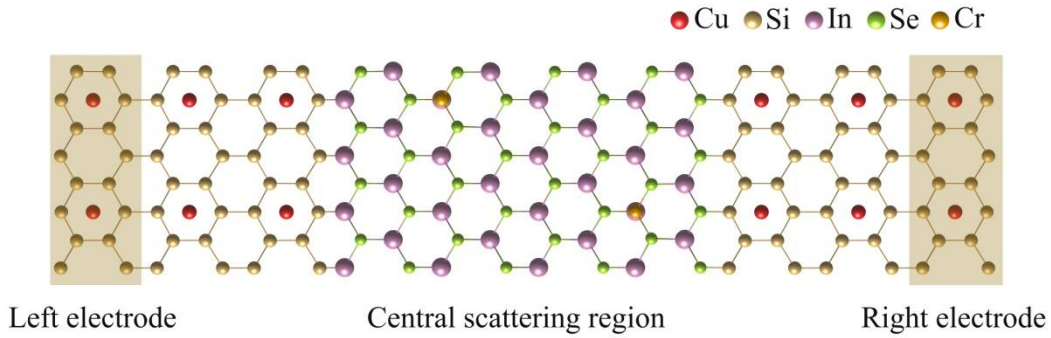

Figure S3. Top view of Cr-InSe device.

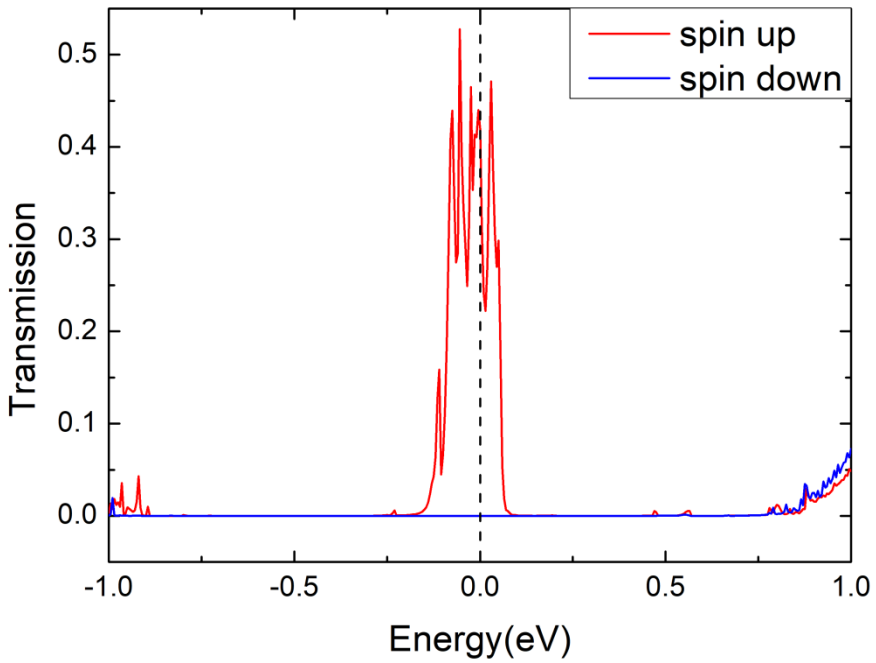

Figure S4. Transmission coefficients of Cr-doped InSe monolayer at zero bias. The blue solid curves and red solid curves correspond to transmission coefficients of spin up state and spin down state, respectively. The vertical dashed line denotes Fermi level