Supplementary Material

Monlayer InSe photodetector with strong anisotropy and surface-bound exciton

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1. Band structure

Fig. S1 compares electronic band structures of monolayer and bulk InSe at the PBE and HSE06 levels. For monolayer InSe, the valence band maximum (VBM) at the PBE (HSE06) level lies between M point and Γ point, whereas the conduction band minimum (CBM) locates at Γ point (M point), presenting an indirect bandgap of 1.4407 eV (3.154 eV). For its bulk counterpart, VBM at the PBE (HSE06) level is at Γ point, while CBM locates at Γ point (M point), which shows a direct (an indirect) bandgap of 0.868 eV (1.663 eV).

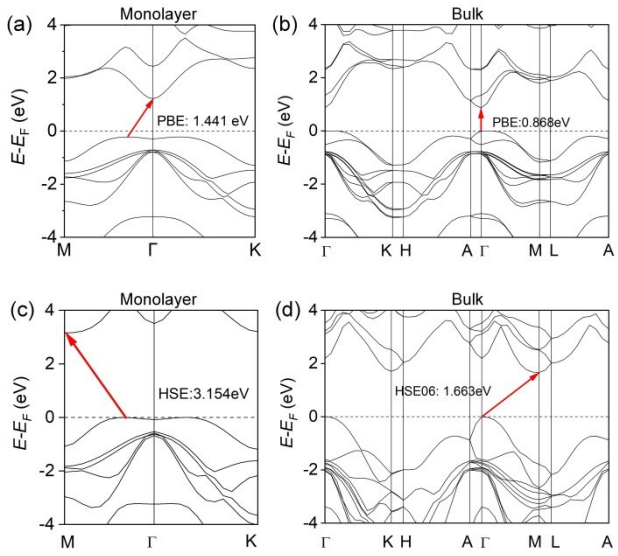

Fig. S1 The band structure of monolayer and bulk InSe using (a-b) PBE and (c-d) HSE06 approaches. Blue rectangle illustrates two pairs of doubly degenerate valence bands of monolayer InSe.

2. Carrier effective mass

To qualitatively investigate the transport property of monolayer InSe, we calculated carrier effective masses along the armchair and zigzag directions of monolayer InSe. Effective masses for electrons (m_e^*) and holes (m_h^*) along the armchair and zigzag directions are acquired through fitting the conduction band minimum (CBM) and the valence band maximum (VBM) along the M → Γ and Γ → K directions based on parabolic functions, respectively, which can be written as[41]:

$$m^* = \pm \hbar \left(\frac{d^2 E_k}{dk^2} \right)^{-1} \qquad (S1)$$

where E_k is the energy at the wave vector **k**. The effective mass for holes m_h of monolayer InSe is 1.07 m_0 (where m_0 is the free electron mass). The effective mass for electrons is predicted to m_e = 0.19 m_0. The predicted m_e along the armchair and zigzag directions of monolayer InSe are 1.11 m_0 and 1.95 m_0. The m_h along the

armchair and zigzag directions are supposed to be 1.90 m_0 and 2.39 m_0. It is obvious that the carrier effective masses along the armchair direction is quite different from those along the zigzag direction, presenting anisotropic transport property of monolayer InSe.

3. Transmission coefficient and partial density of states

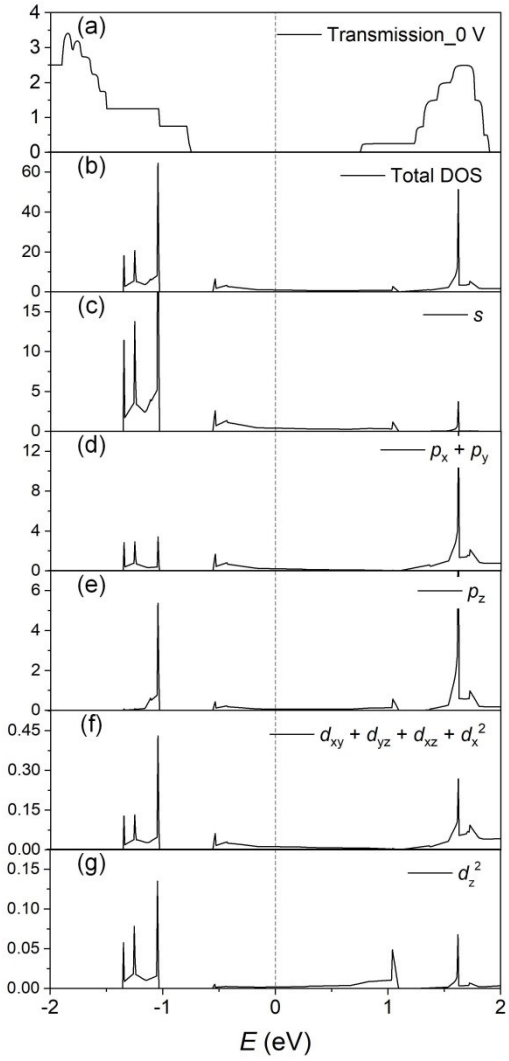

Fig. S2 (a) The transmission coefficient as a function of electron energy in the armchair direction of monolayer InSe photodetector at 0 V. (b) The total density of state and (c-g) partial density of state of monolayer InSe.

4. The photocurrent in the extinction ratio

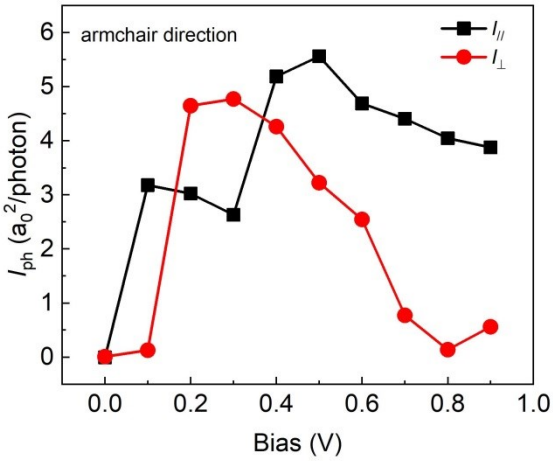

Fig. S3 The variation in I_{ph} with the source-drain bias voltage of monolayer InSe in the armchair direction.