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Electronic Supplementary Information for

Enhancement of photoluminescence and hole mobility in 1- to 5-layer InSe due to the top valence-band inversion: strain effect

Meng Wu,[a] Jun-jie Shi,*[a] Min Zhang,[b] Yi-min Ding,[a] Hui Wang,[a] Yu-lang Cen[a] and Jing Lu[a]

[a] State Key Laboratory for Artificial Microstructures and Mesoscopic Physics, School of Physics, Peking University, Beijing 100871, China. E-mail: jjshi@pku.edu.cn

[b] College of Physics and Electronic Information, Inner Mongolia Normal University, Hohhot 010022, China

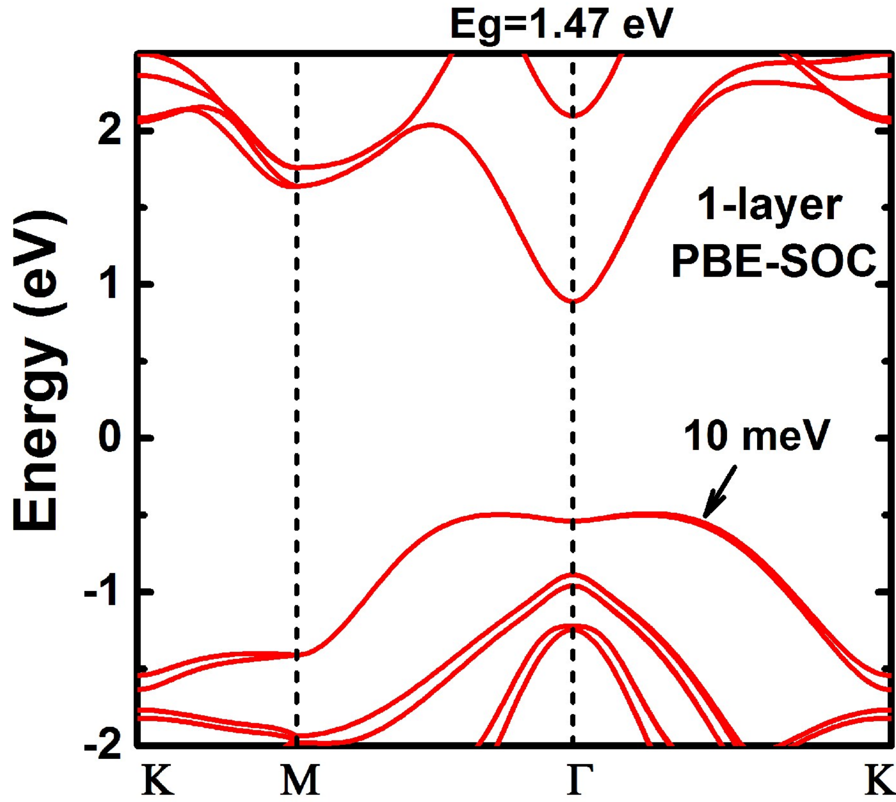

Fig. S1 Electronic band structure of InSe monolayer derived from GGA-PBE calculations, in which the SOC effect is included. We find that the spin splitting at VBM is just 10 meV. This means that the SOC is quite weak and can be negligible in 2D InSe materials, which has also been confirmed by some previous works.[1-3] Compared with Fig. 2(b), the bandgap, band symmetry and PL spectra have no any detectable variation due to the ignorable splitting caused by the SOC effect.

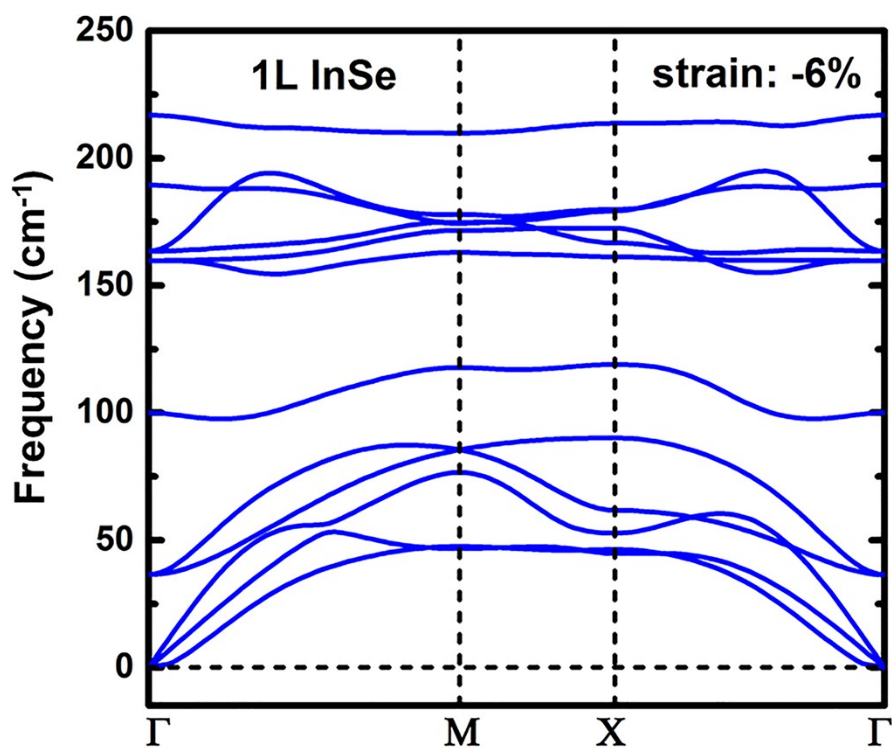

Fig. S2 Calculated phonon dispersions of monolayer InSe under 6% compressive strain. All phonon frequencies are positive and no imaginary frequency phonon modes are observed. This clearly proves that 1-layer InSe with -6% strain is stable.

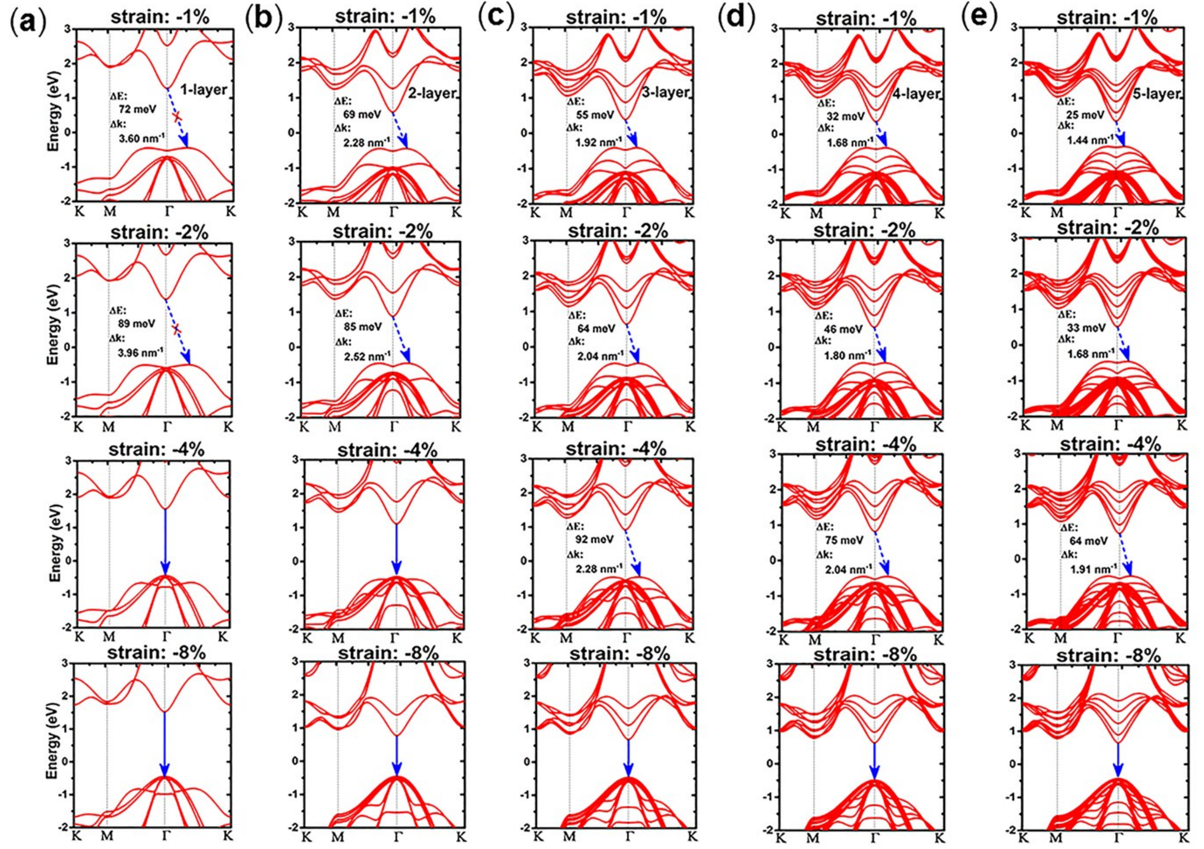

Fig. S3 Evolution of the electron band structures of (a) 1- to (e) 5-layer InSe under the compressive strains of 1%, 2%, 4% and 8%, respectively. The ΔE and Δk denote the energy and wavenumber difference between VBM and Γ point.

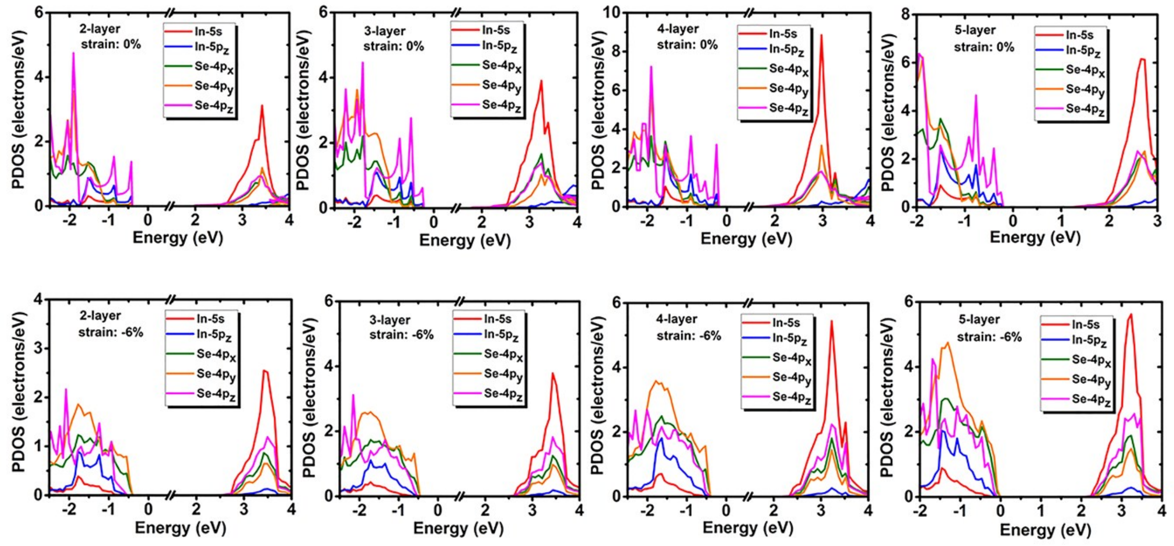

Fig. S4 PDOSs of 2- to 5-layer InSe under freestanding and 6% compressive strain conditions. Here, the PDOSs of In $5p_x$, $5p_y$ and Se 4s orbitals are small and have been neglected for clarity.

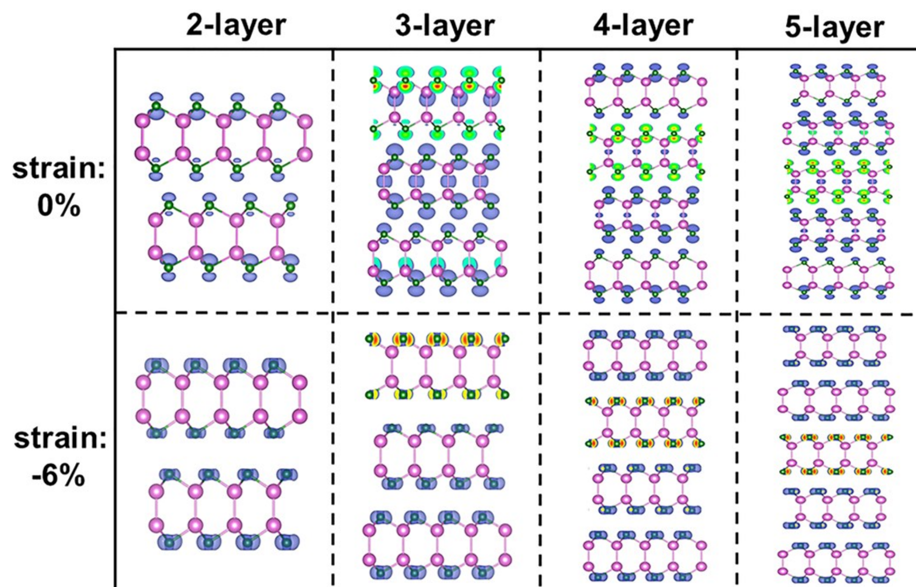

Fig. S5 Isosurface charge density distributions (ρ=0.008 $eÅ^{-3}$) at VBM for 2- to 5-layer InSe under freestanding and 6% compressive strain conditions.

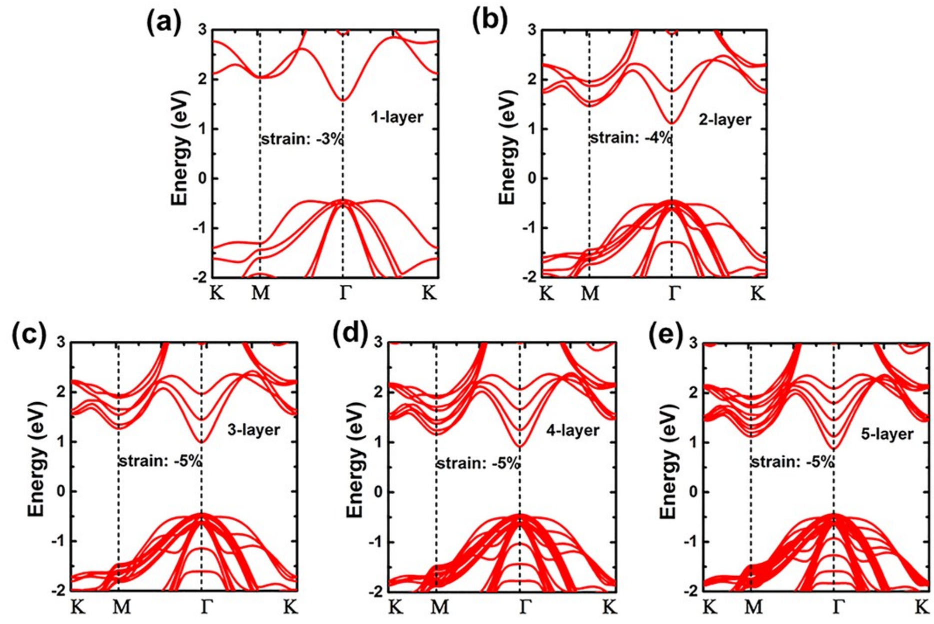

Fig. S6 The strain-modified band structures for (a) 1- to (e) 5-layer InSe at the indirect-to-direct bandgap transition points with the compressive strain of 3% for monolayer, 4% for bilayer, and 5% for 3-, 4- and 5-layer InSe.

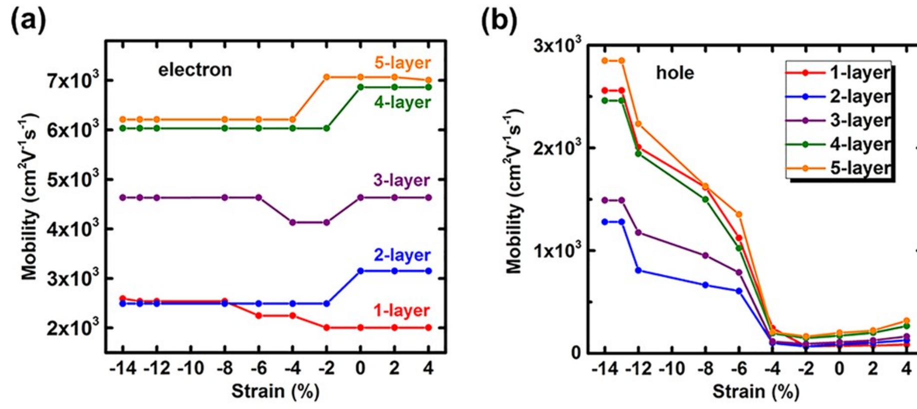

Fig. S7 Dependence of electron (a) and hole (b) mobility on strain in 1- to 5-layer InSe. The electron mobility (~10^3 $cm^2V^{-1}s^{-1}$) increases with the layer-thickness and is insensitive to strain. On the contrary, the hole mobility has a remarkable increase under the compressive strain and approaches its maximum ~10^3 $cm^2V^{-1}s^{-1}$ at about -13% strain.

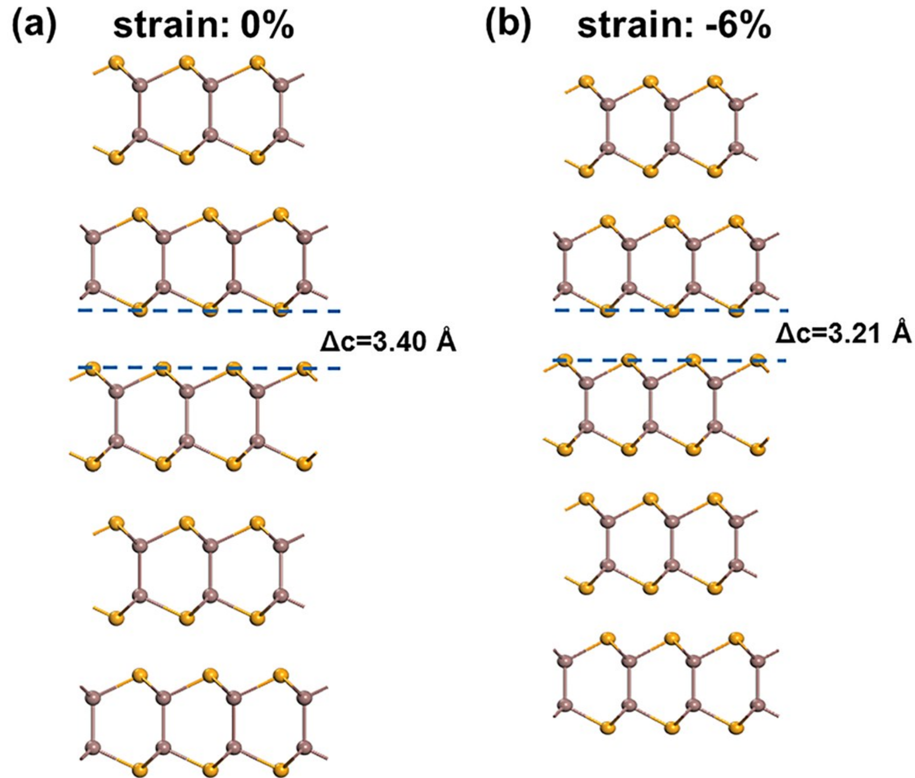

Fig. S8 The optimized structures for 5-layer InSe (a) without strain and (b) with 6% compressive strain. The calculated average interlayer distance (Δc) is 3.40 (3.21) Å for the freestanding (strained) InSe. We can find that Δc is larger than the Se-Se covalent bond length (~2.32 Å). Hence, no chemical bonds are formed between the two InSe sub-layers under 6% compressive strain.

References

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