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

Strain induced new Phase and Indirect-Direct Band Gap Transition of Monolayer InSe

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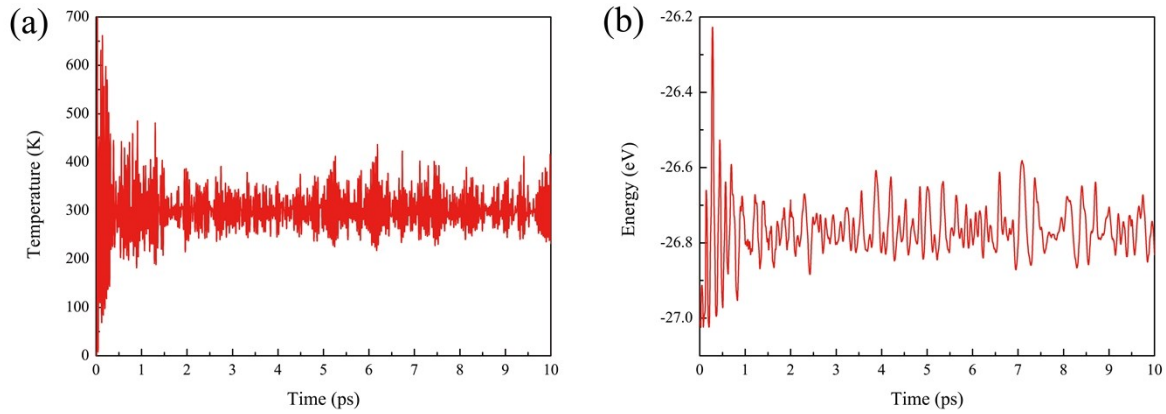

Fig. S1 Fluctuations of (a) temperature and (b) total energy as a function of the molecular dynamics simulation step at 300 K.

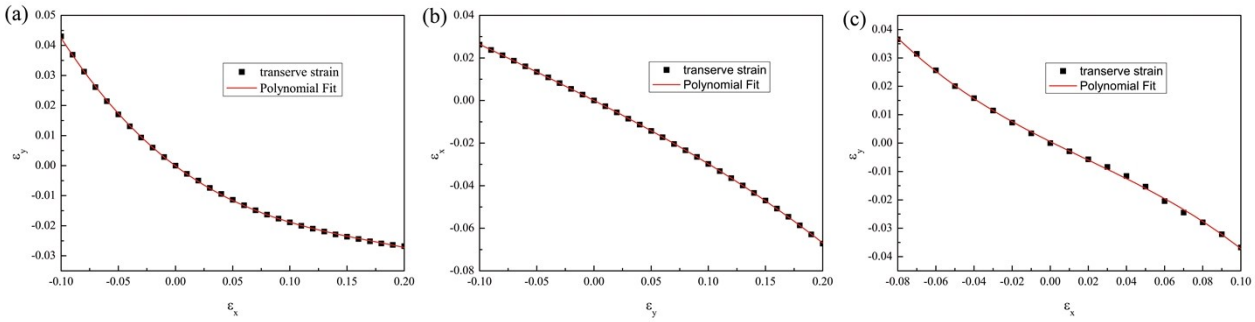

Fig. S2 (a)The in-plane Poisson's ratio ε_y versus ε_x under uniaxial strain ε_x for phase-I InSe. Data are fitted to function y= -0.284x+1.191x^2-2.245x^3. (b) ε_x versus ε_y under uniaxial strain ε_y for phase-I InSe. Data are fitted to function y=-0.274x-0.169x^2-0.672x^3. (c) ε_y versus ε_x under uniaxial strain ε_x for phase-II InSe. Data are fitted to function y= -0.335x+0.649x^2-10.68x^3.

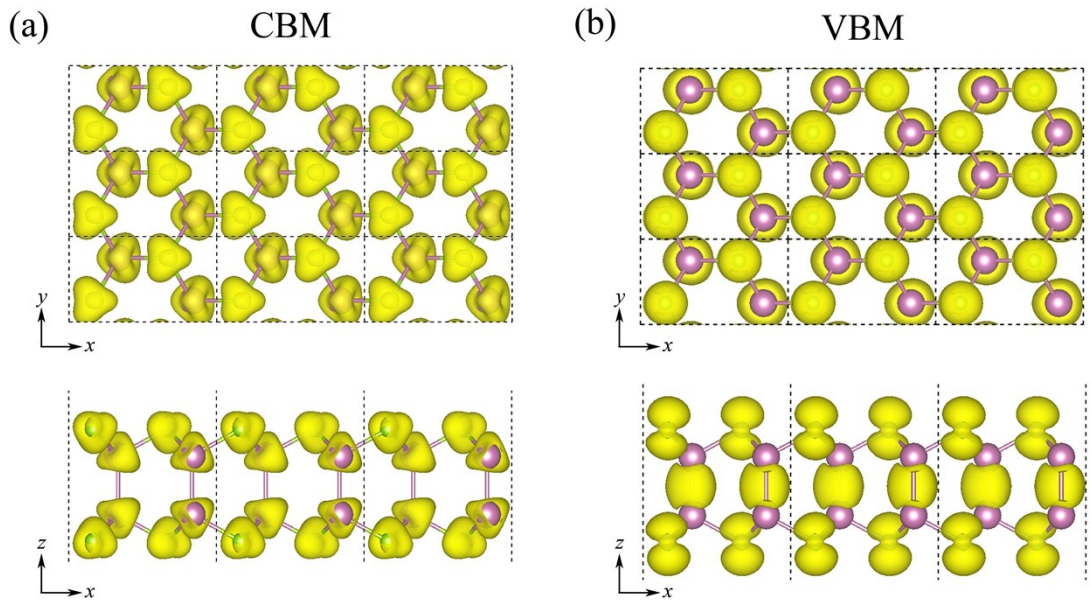

Fig. S3 The partial charge densities of (a) CBM and (b) VBM.