Electronic Supplementary Information for the paper:

"Indium Selenide Monolayer: A Two-Dimensional Material with Strong Second Harmonic Generation"

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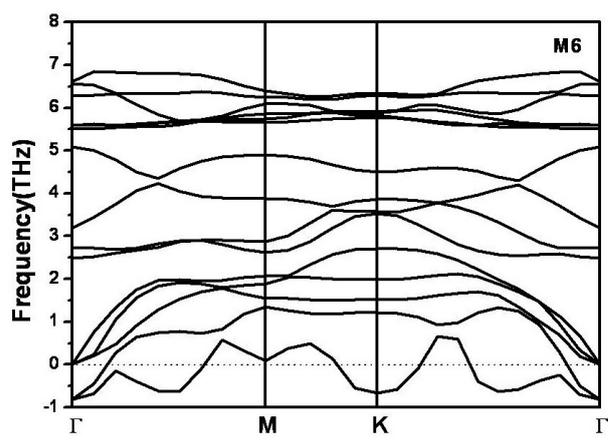[b] *Department of Physics, Zunyi Normal University, Zunyi, Guizhou, 563006, China*
[c] *Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry, Xiamen, Fujian, 361005, China*
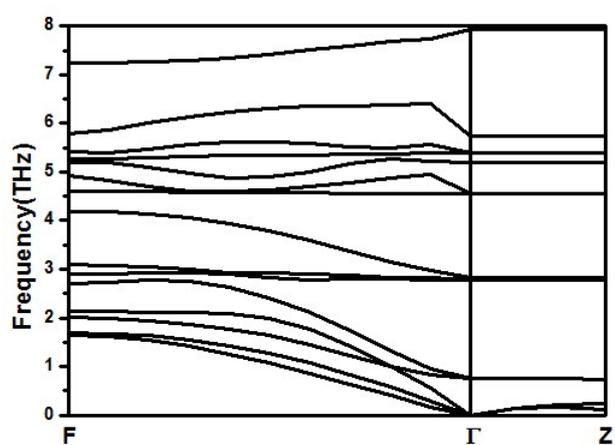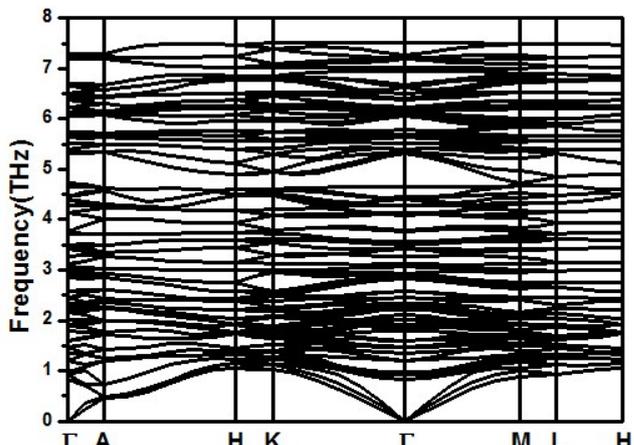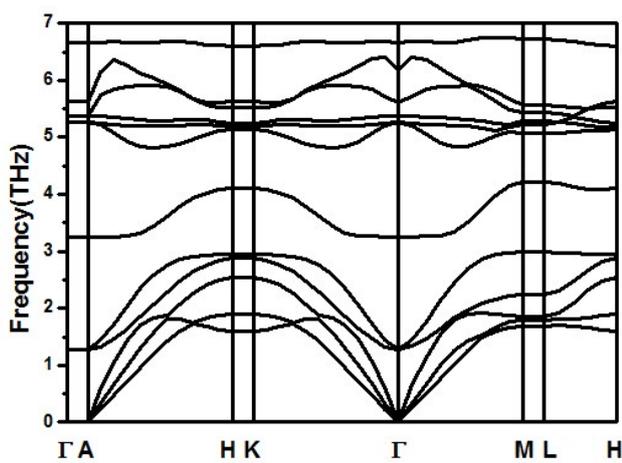* E-mail: zhangyf@fzu.edu.cn
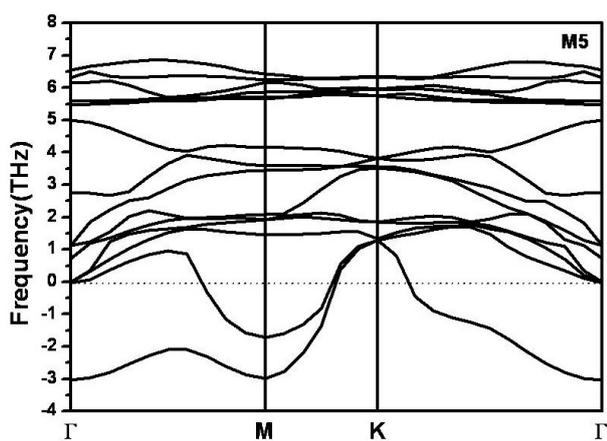
(a) M5 model

(b) M6 model

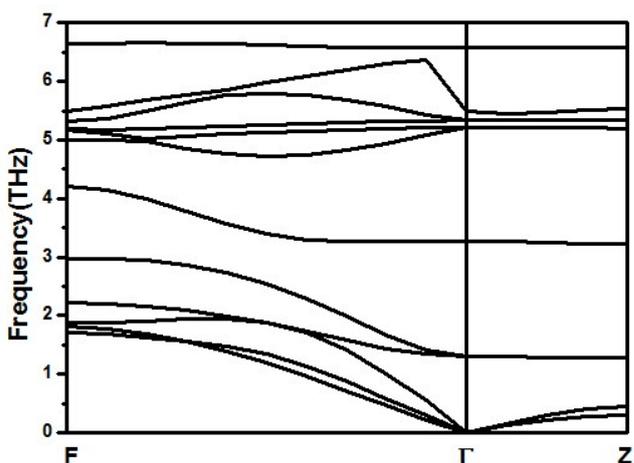Figure S1 The calculated phonon spectra of (a) M5 model and (b) M6 model

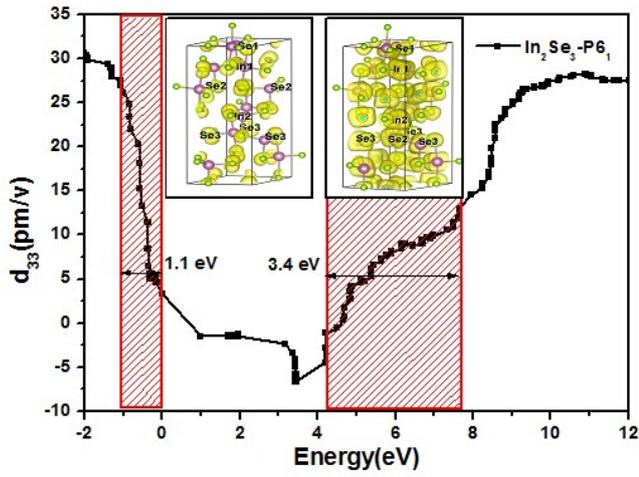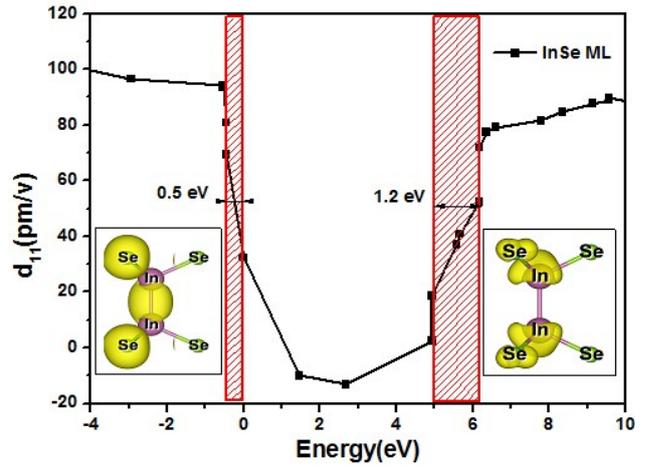(a) In_2Se_3-R3m

(b) In_2Se_3-P6_1

(c) InSe ML

(d) InSe-R3m

Figure S2 The calculated phonon spectra of different In-Se compounds including (a) In_2Se_3-R3m, (b) In_2Se_3-P6$_1$, (c) InSe ML, (d) InSe-R3m.

(a) In$_2$Se$_3$-P6$_1$ (b) InSe ML

Figure S3 Variation of static SHG coefficient as a function of the cutoff energy of (a) In$_2$Se$_3$-P6$_1$, and (b) InSe-ML. The partial charge density maps shown in the insets of (a) are drawn by considering bands in the energy regions from -1.1 eV to VBM and from 4.2 to 7.7 eV, respectively, while in (b) the corresponding energy regions are from -0.5 eV to VBM and from 5.0 to 6.2 eV, respectively.