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

Exotic magnetism in As-doped α/β-In_2Se_3 monolayers with tunable anisotropic carrier mobility

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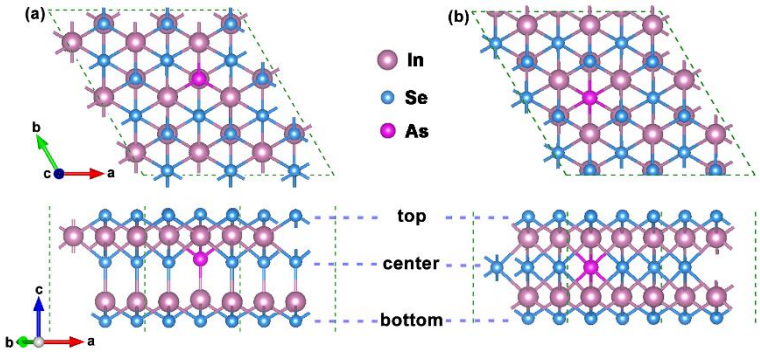

Figure S1 Top (upper panels) and side (lower panels) views of an arsenic substitution on the Se site (As_{Se}) in α-In_2Se_3 (left panels) and β-In_2Se_3 (right panels), respectively. The layers of Se sites located are indicated by top, center and bottom.

In the 3×3 supercell, one Se atom is replaced by one As atom. Because the Se atoms on different layers show different valence, three configurations are considered, i.e., the defect on the top layer ($As_{Se\text{-}top}$), center layer ($As_{Se\text{-}center}$) and bottom layer ($As_{Se\text{-}bottom}$).

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Table S1 The formation energies of α/β-In_2Se_3 and they with As_{Se} defects.

	Formation energy (eV/Å^2)
α-In_2Se_3	-0.1784
α-In_2Se_3 with $As_{Se\text{-}top}$	-0.1635
α-In_2Se_3 with $As_{Se\text{-}center}$	-0.1665
α-In_2Se_3 with $As_{Se\text{-}bottom}$	-0.1687
β-In_2Se_3	-0.1788
β-In_2Se_3 with $As_{Se\text{-}top}$	-0.1637
β-In_2Se_3 with $As_{Se\text{-}center}$	-0.1658
β-In_2Se_3 with $As_{Se\text{-}bottom}$	-0.1638

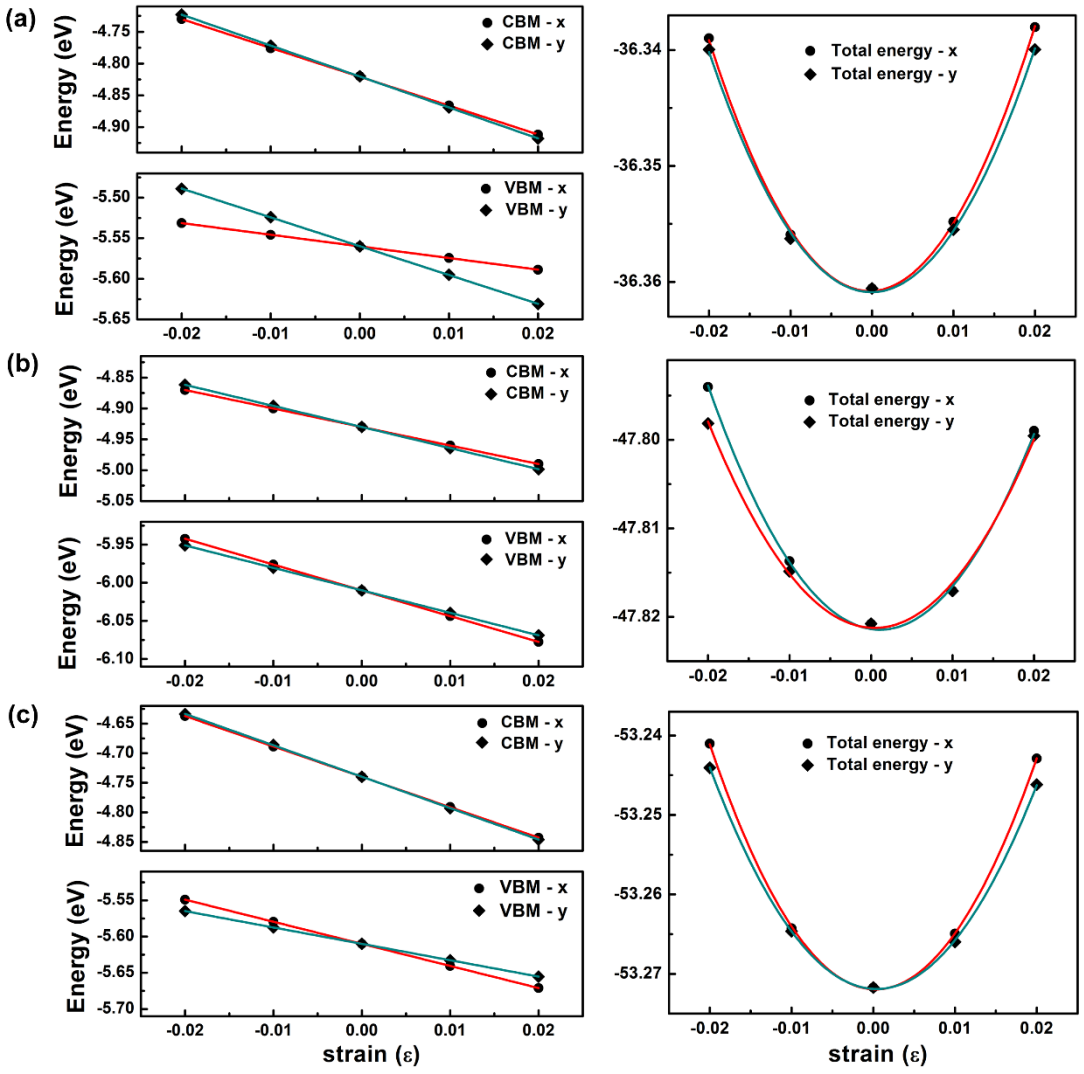

Figure S2. Linear fitting of band edges and quadratic fitting of total energy as a function of uniaxial strain for (a) α-In_2Se_3 (b) α-In_2Se_3-O_2 (c) α-In_2Se_3-H_2O monolayers.

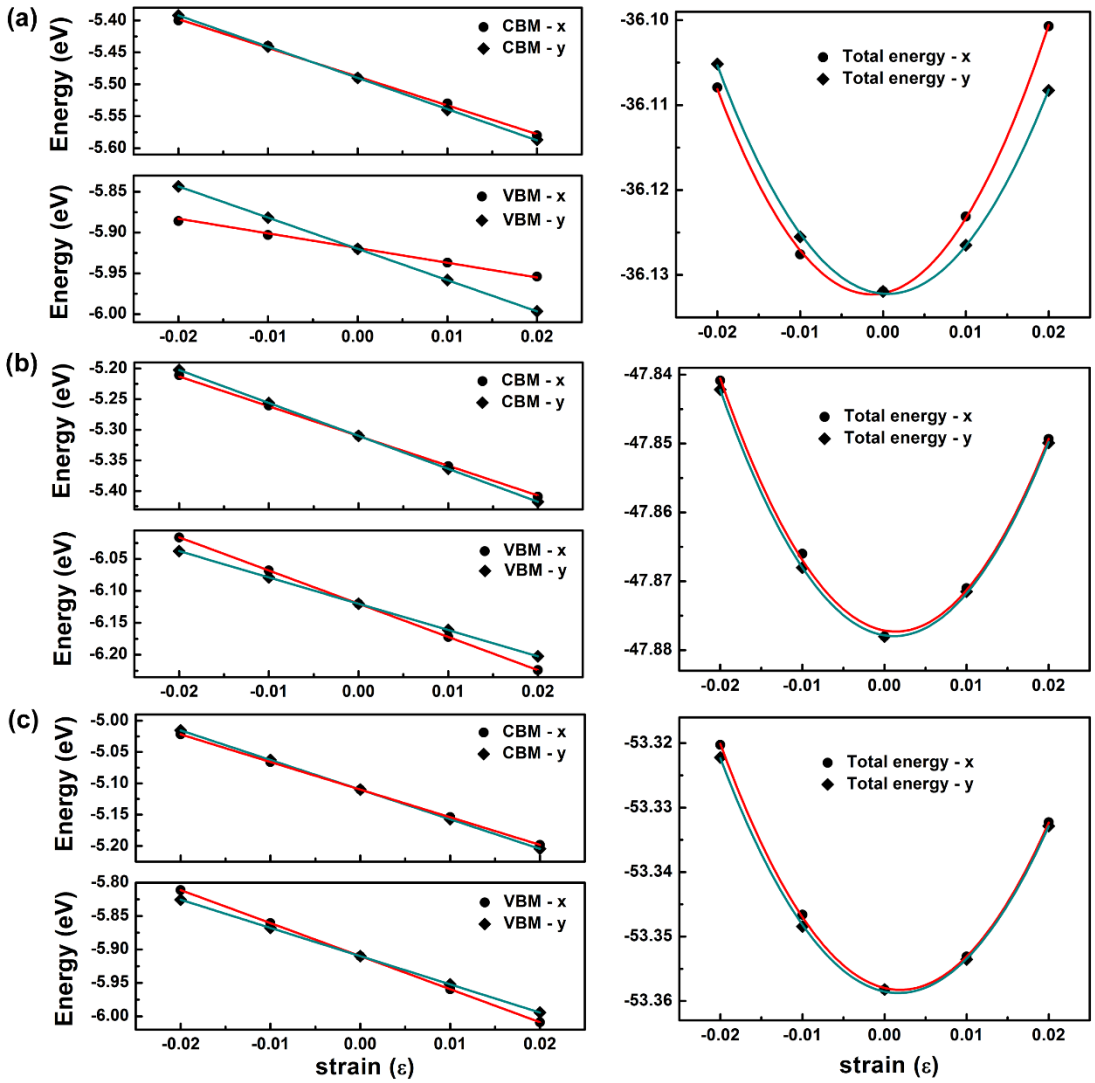

Figure S3. Linear fitting of band edges and quadratic fitting of total energy as a function of uniaxial strain for (a) β-In_2Se_3 (b) β-In_2Se_3-O_2 (c) β-In_2Se_3-H_2O monolayers.