Electronic Supplementary Material (ESI) for Nanoscale.

Quantum Spin Hall Insulators in Functionalized Arsenene (AsX, X=F, OH and CH_3) Monolayers with Pronounced Light Absorption

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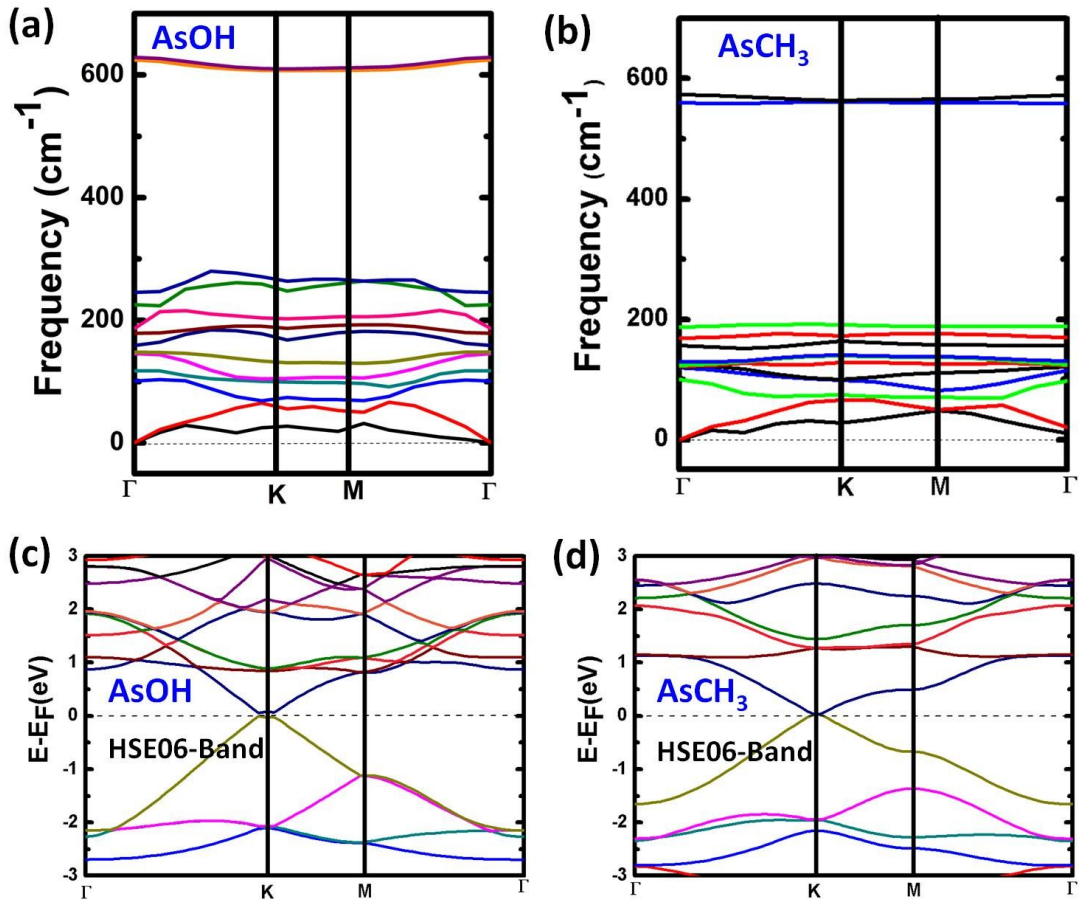

Fig. S1 The phonon spectra along highly symmetrical points in the BZ for the (a) AsOH and (b) $AsCH_3$ functionalized configurations. The calculated electronic band structures with HSE06 functional for the (c) AsOH and (d) $AsCH_3$ functionalized configurations.

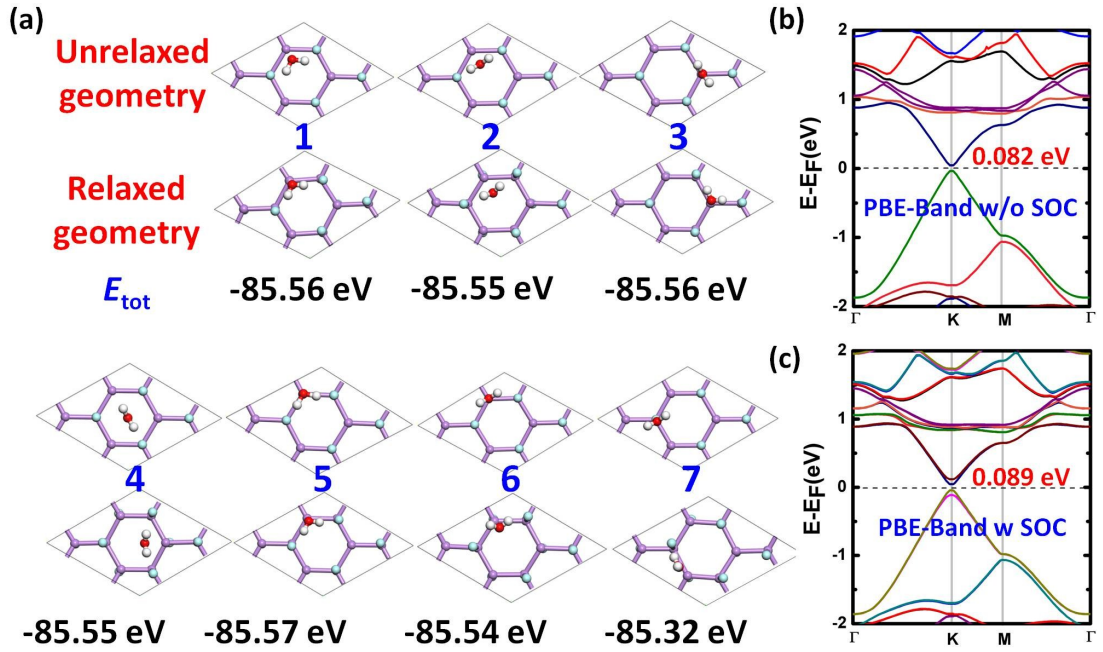

Fig. S2 Various conformations (a) for an adsorption of single water molecules on the surface of AsF chemical functionalization, with corresponding total energies denoted in the Figure. The calculated band structures without SOC and with SOC are shown in (b) and (c).

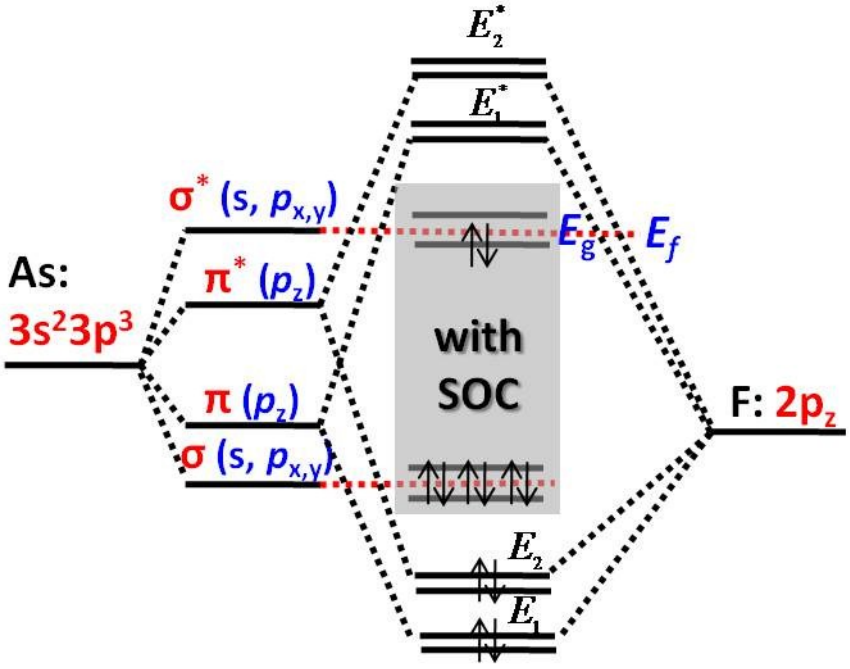

Fig. S3 The schematic diagram of the band evolution for AsF monolayer with SOC effect. The black arrows refer to the occupied electrons. The Fermi level E_f is indicated by the red dashed line.

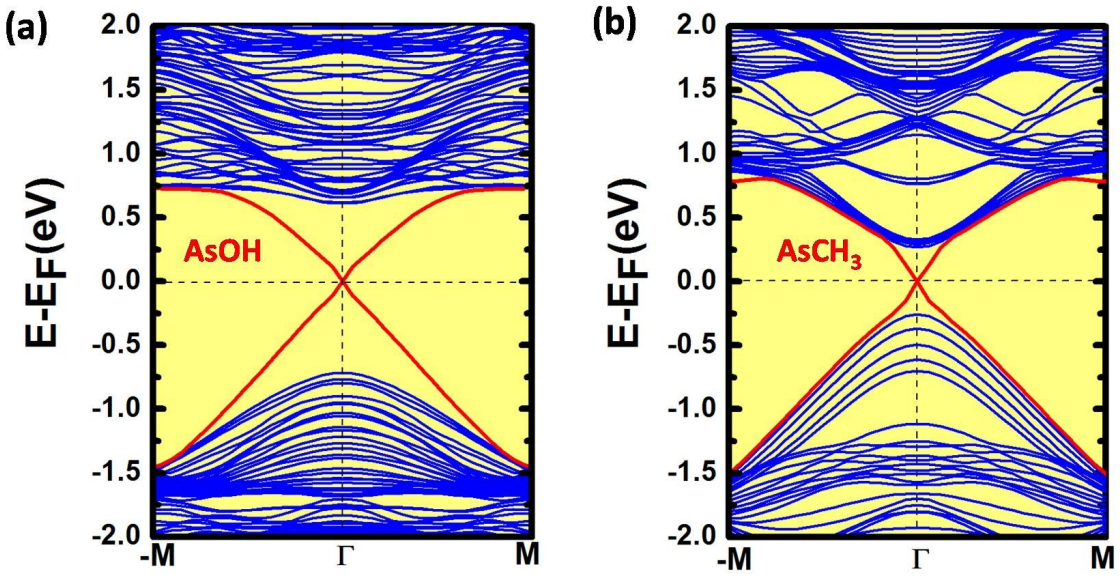

Fig. S4 Calculated edge states for the (a) AsOH functionalized configuration and (b) $AsCH_3$ functionalized configuration.

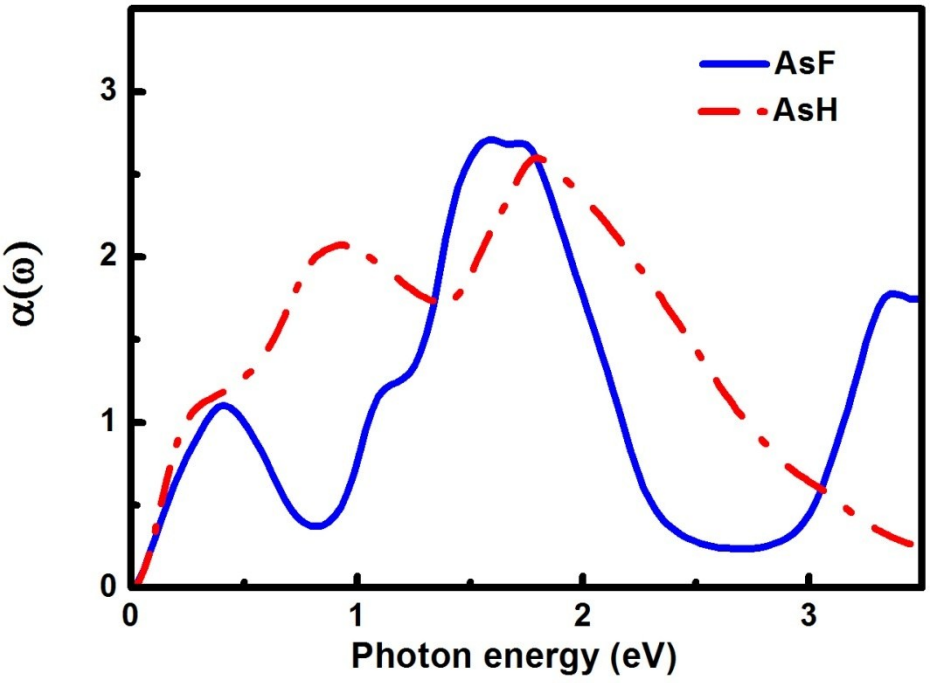

Fig. S5 Absorbance coefficients for AsF and AsH monolayers.