Supporting information

First-principles investigation of ScX_2 (X = Cl, Br or I) monolayers for flexible spintronics and electronics

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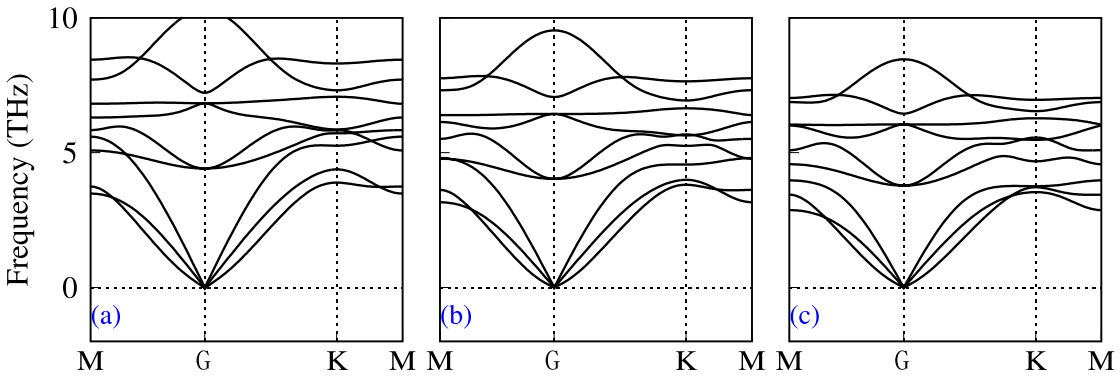

Figure S1. Phonon spectra for the (a) 1H-$ScCl_2$, (b) 1H-$ScBr_2$, (c) 1H-ScI_2, respectively.

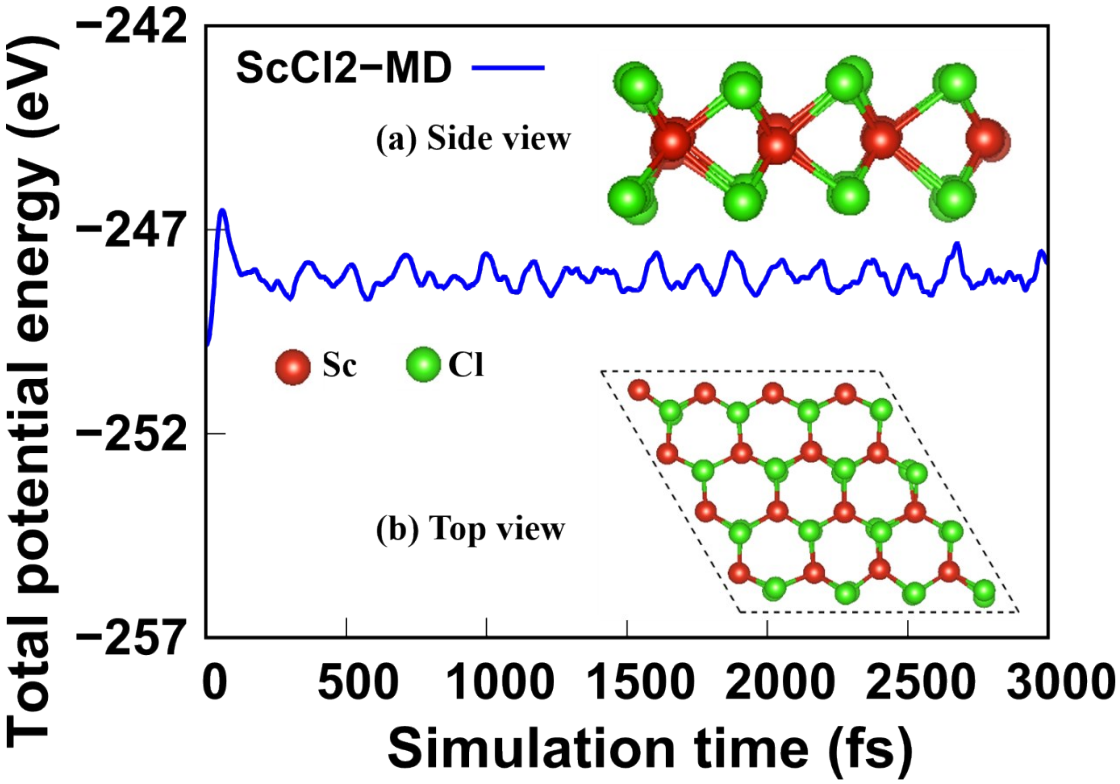

Figure S2. Potential energy of $ScCl_2$ monolayer as a function of time step within the canonical ensemble at T = 300 K.

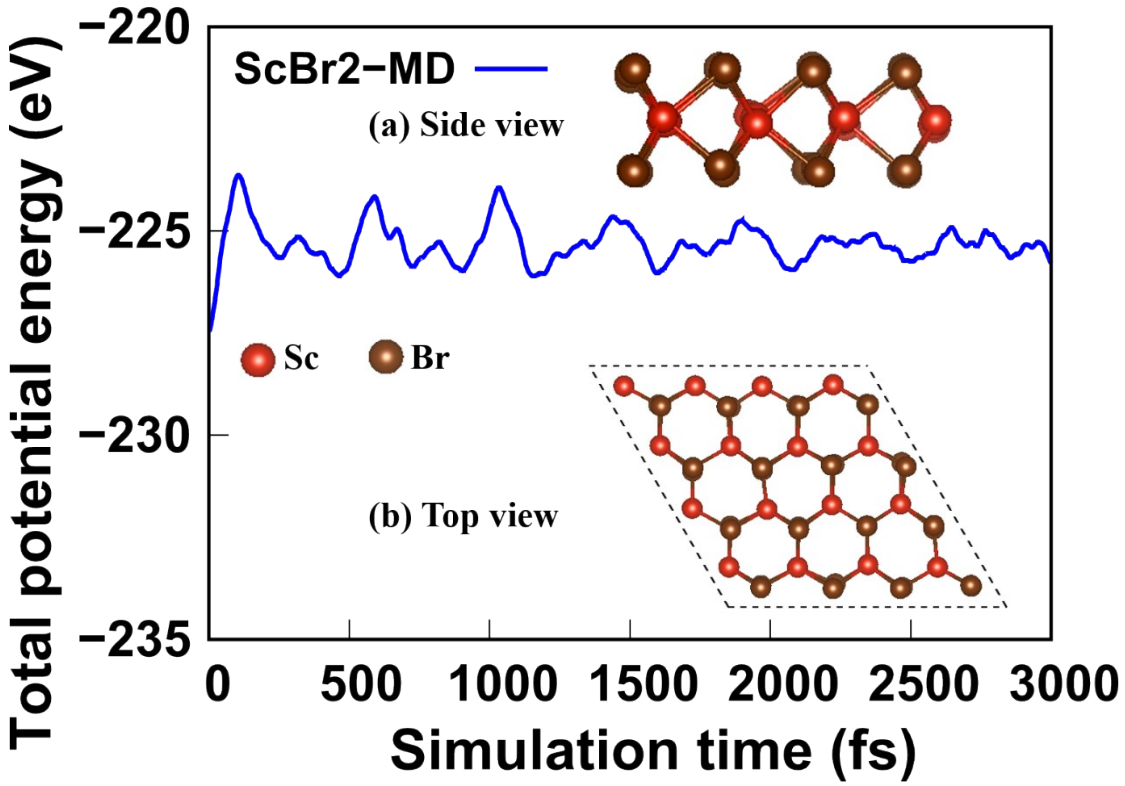

Figure S3. Potential energy of $ScBr_2$ monolayer as a function of time step within the canonical ensemble at T = 300 K.

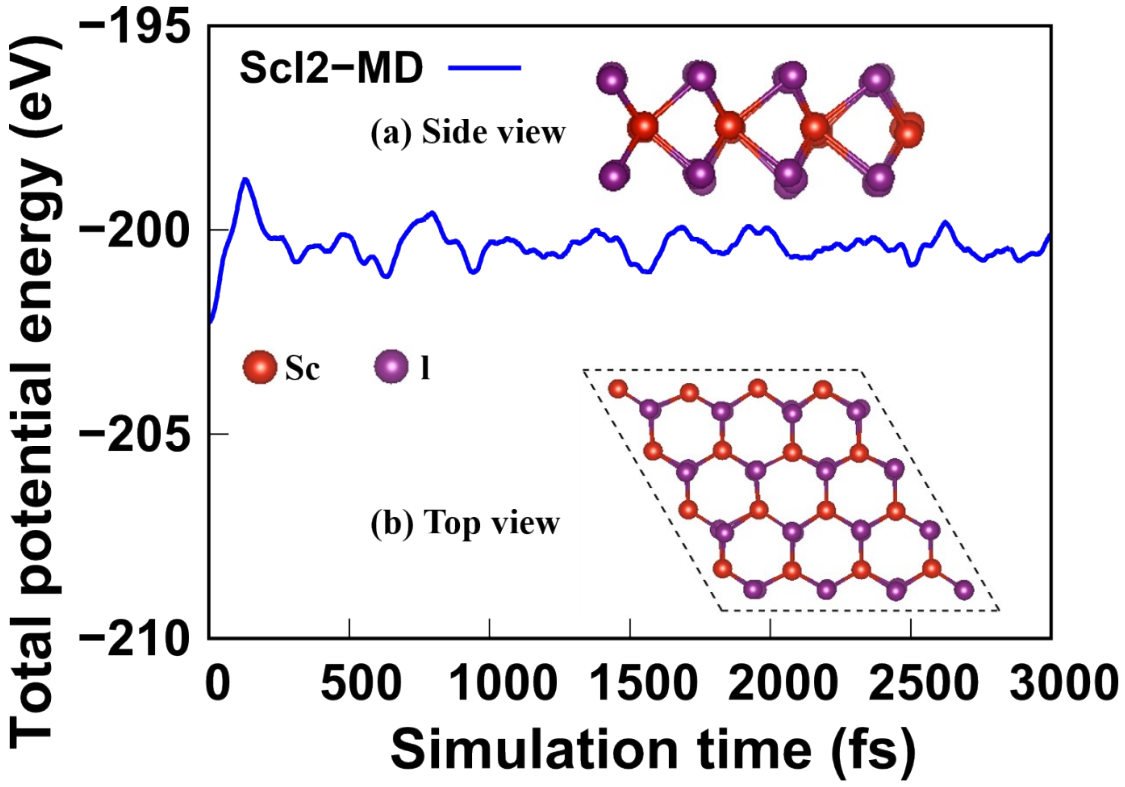

Figure S4. Potential energy of ScI_2 monolayer as a function of time step within the canonical ensemble at T = 300 K.

Table S1 Elastic constants for ScX_2 (X = Cl, Br or I) monolayers.

Systems	C_{11} (N/m)	C_{12} (N/m)	C_{44} (N/m)
$ScCl_2$	56	14	20
$ScBr_2$	50	14	18
ScI_2	42	10	16

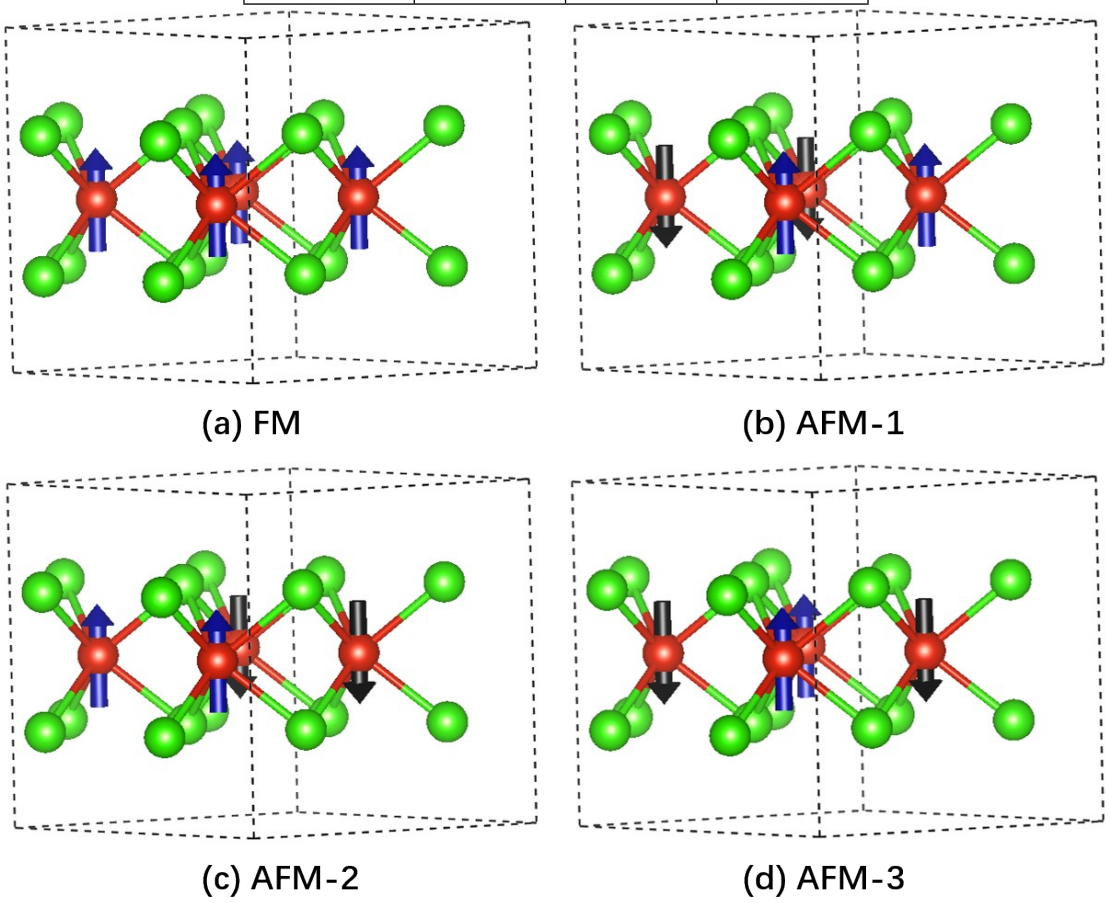

Figure S5. Configurations of the magnetic structures: (a) Ferromagnetic structure, (b) type-1 antiferromagnetic structure, (c) type-2 antiferromagnetic structure, and (d) type-3 antiferromagnetic structure.

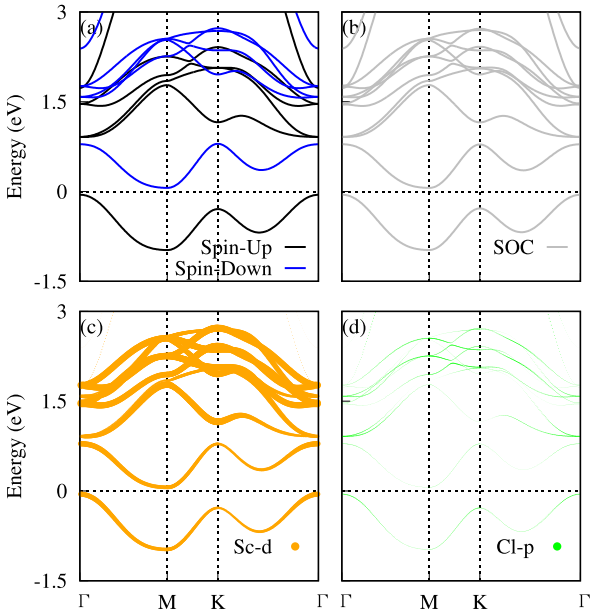

Figure S6. Calculated band structure of the $ScCl_2$ monolayer: (a) without SOC effect; (b) with SOC effect; (c) contributions of the d orbitals of the Sc elements to the band structure; (d) contributions of the p orbitals of the Cl elements to the band structure.

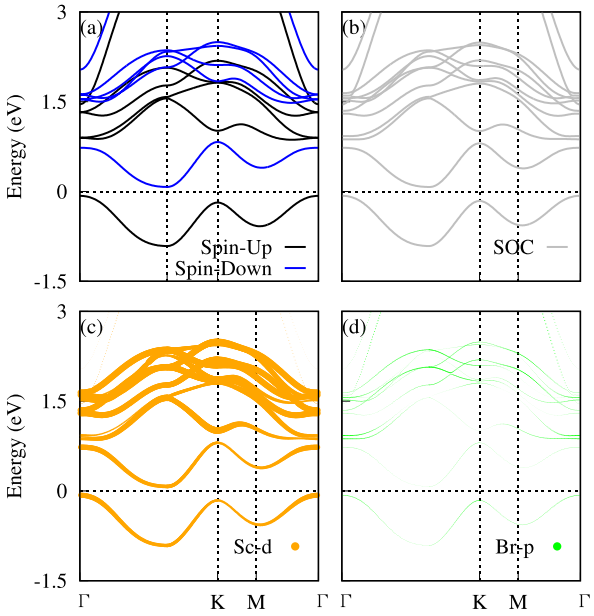

Figure S7. Calculated band structure of the $ScBr_2$ monolayer: (a) without SOC effect; (b) with SOC effect; (c) contributions of the d orbitals of the Sc elements to the band structure; (d) contributions of the p orbitals of the Br elements to the band structure.

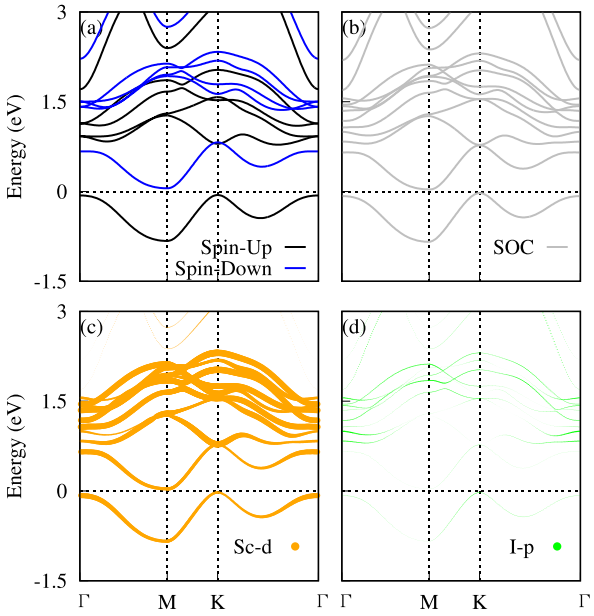

Figure S8. Calculated band structure of the ScI_2 monolayer: (a) without SOC effect; (b) with SOC effect; (c) contributions of the d orbitals of the Sc elements to the band structure; (d) contributions of the p orbitals of the I elements to the band structure.

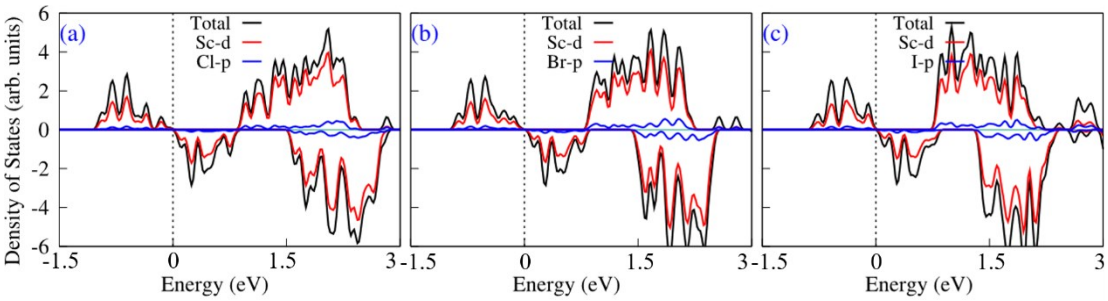

Figure S9. Partial and total density of states for the (a) $ScCl_2$, (b) $ScBr_2$, and (c) ScI_2 monolayers, respectively.

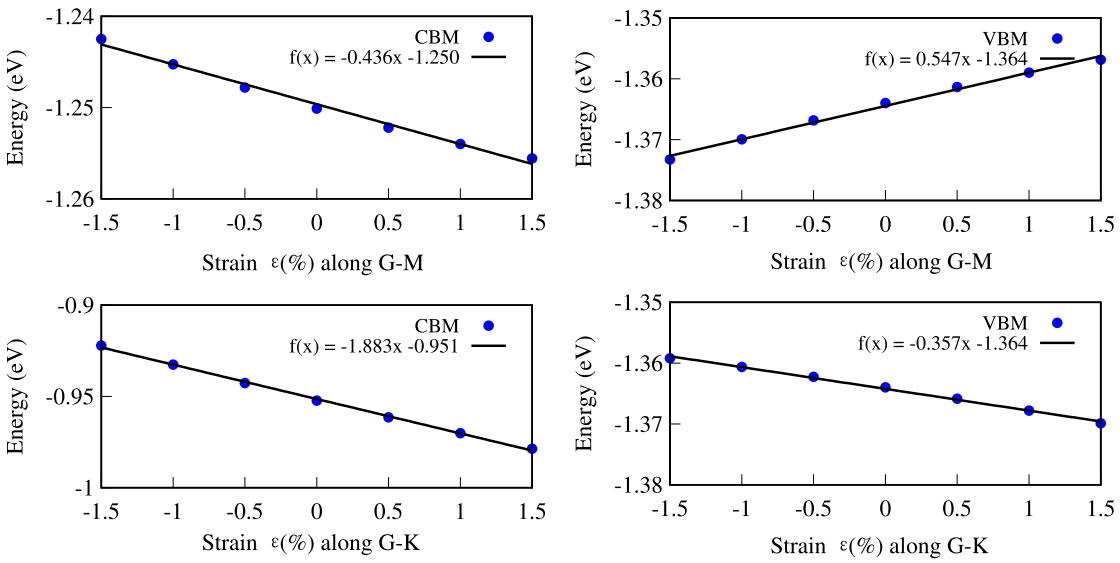

Figure S10. Band energies of the Conduction Band Minimum (CBM) and Valence Band Maximum (VBM) for $ScCl_2$ monolayer, with respect to uniaxial compression or tension along the G-M and G-K directions, respectively. Blue points represent CBM or VBM, whereas black lines mean the fitting curves.

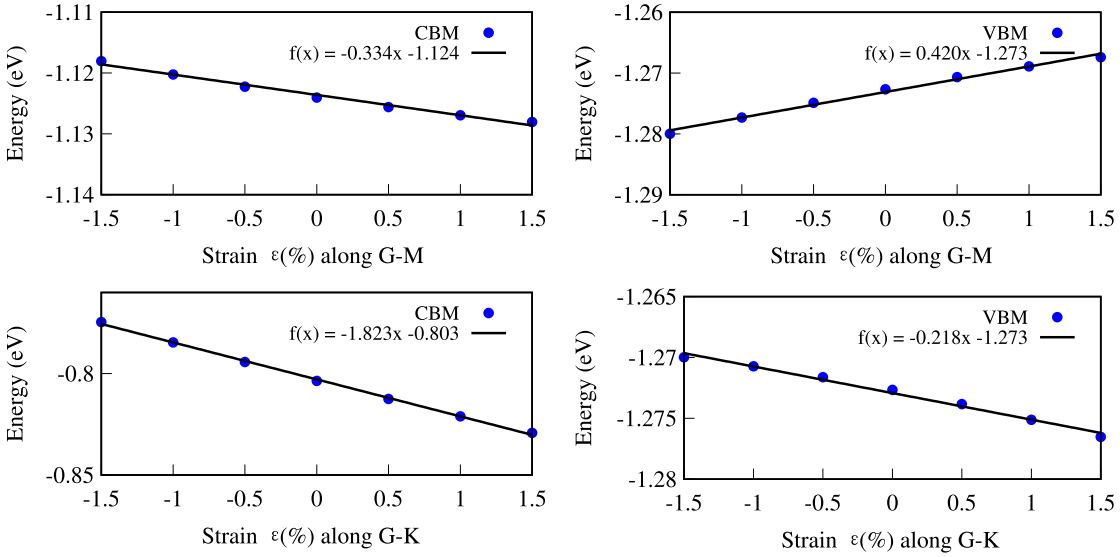

Figure S11. Band energies of the Conduction Band Minimum (CBM) and Valence Band Maximum (VBM) for $ScBr_2$ monolayer, with respect to uniaxial compression or tension along the G-M and G-K directions, respectively. Blue points represent CBM or VBM, whereas black lines mean the fitting curves.

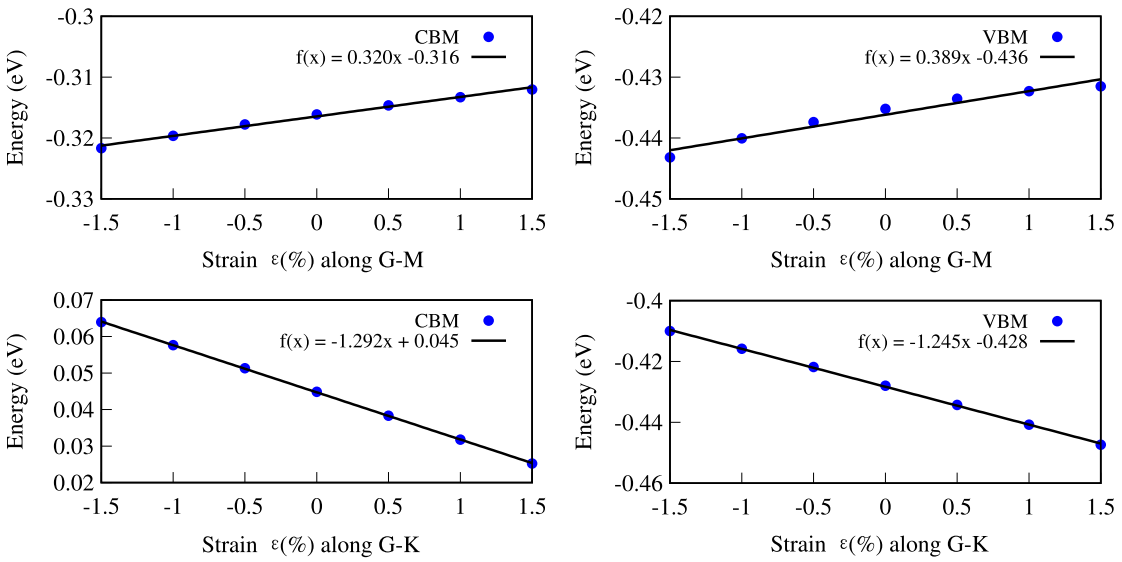

Figure S12. Band energies of the Conduction Band Minimum (CBM) and Valence Band Maximum (VBM) for ScI_2 monolayer, with respect to uniaxial compression or tension along the G-M and G-K directions, respectively. Blue points represent CBM or VBM, whereas black lines mean the fitting curves.