Supporting Information

Strain-Tunable Electric Structure and Magnetic Anisotropy in Monolayer CrSI

Ruilin Han, *[a] and Yu Yan[b]

a School of Physics and Electronic Engineering, Shanxi University, Taiyuan 030006, China

b *Key Laboratory of Physics and Technology for Advanced Batteries (Ministry of Education), Department of Physics, Jilin University, Changchun* 130012*, China*

Figure S1. (a) Total DOS and partial DOS of p orbitals of the I atom, p orbitals of S atom, and d orbitals of Cr atom for the unstrained monolayer CrSI. (b) Spin-up and (c) Spin-down band structures for the unstrained monolayer CrSI. The Fermi energy is indicated by the dashed vertical line.

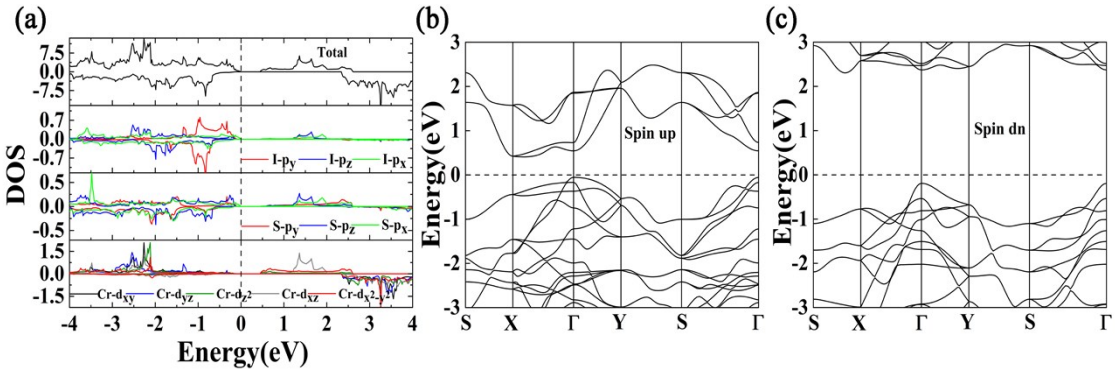

Figure S2. 2×2×1 supercells of monolayer CrSI with (a) FM and (b-f) five different antiferromagnetic states. The arrows represent the spin orientation of Cr atoms. The gray, yellow and red balls represent Cr, S and I atoms, respectively.

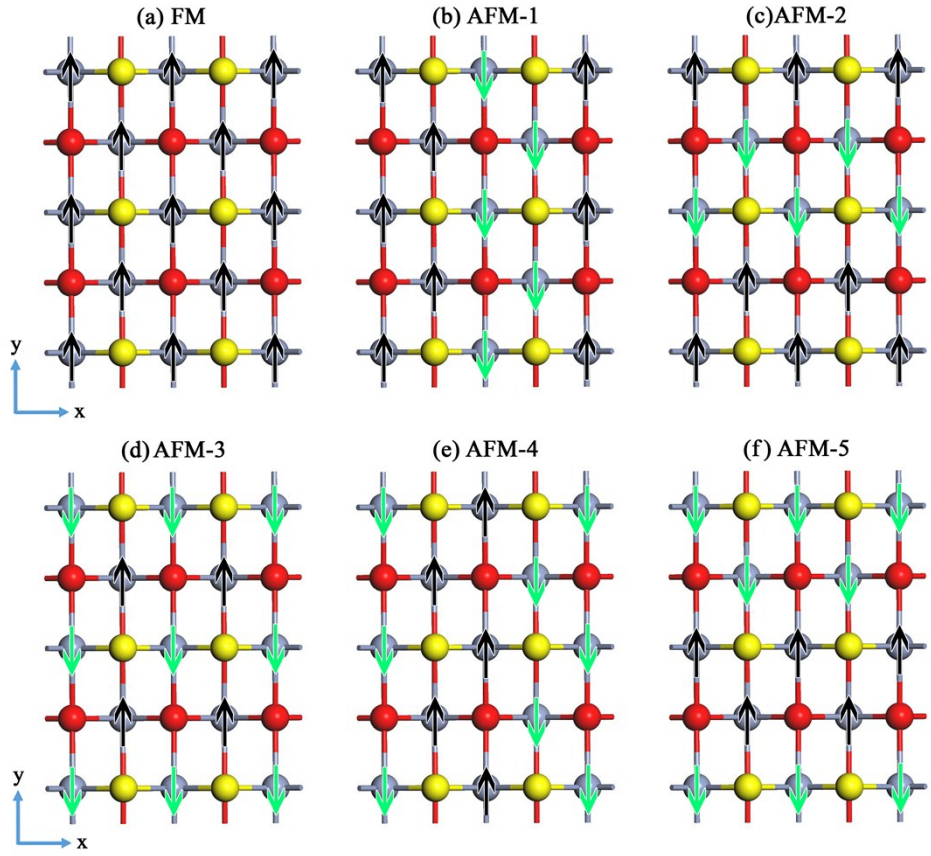

Figure S3. The p orbital-resolved MAE of I atom for the unstrained monolayer CrSI when (a) angle θ is equal to 0° and (b) angle θ is equal to 90°.