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

Supporting information

Two-dimensional pentagonal CrX (X = S, Se or Te) monolayers: Antiferromagnetic semiconductors for spintronics and photocatalysts

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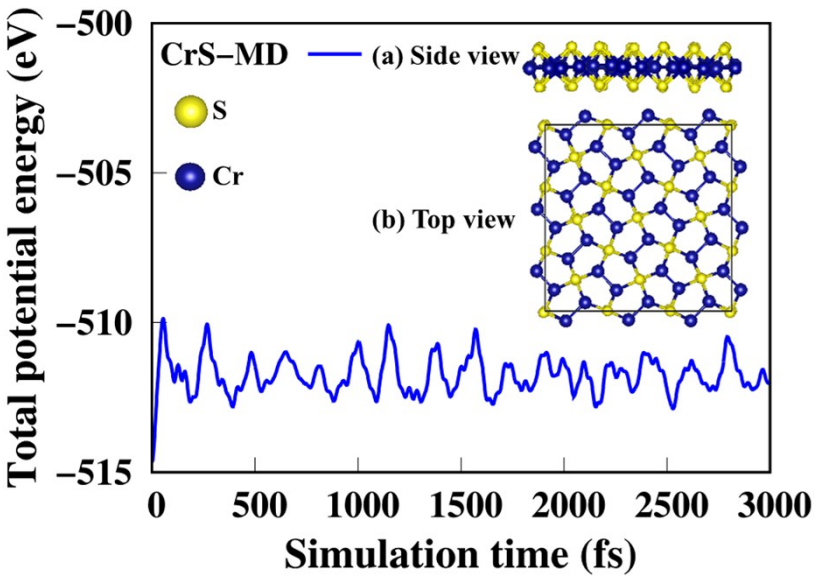

Figure S1. Total potential energy of penta-CrS monolayer as a function of simulation time within canonical ensemble at a constant temperature of 300K. The insets are the (a) side and (b) top views of the configuration after 3 ps (3000 fs).

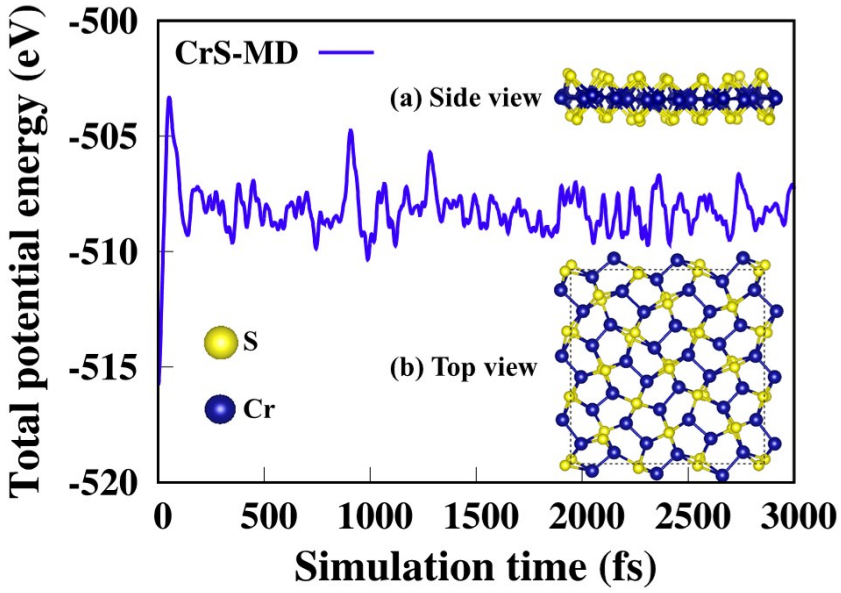

Figure S2. Total potential energy of penta-CrS monolayer as a function of simulation time within canonical ensemble at a constant temperature of 800K. The insets are the (a) side and (b) top views of the configuration after 3 ps (3000 fs).

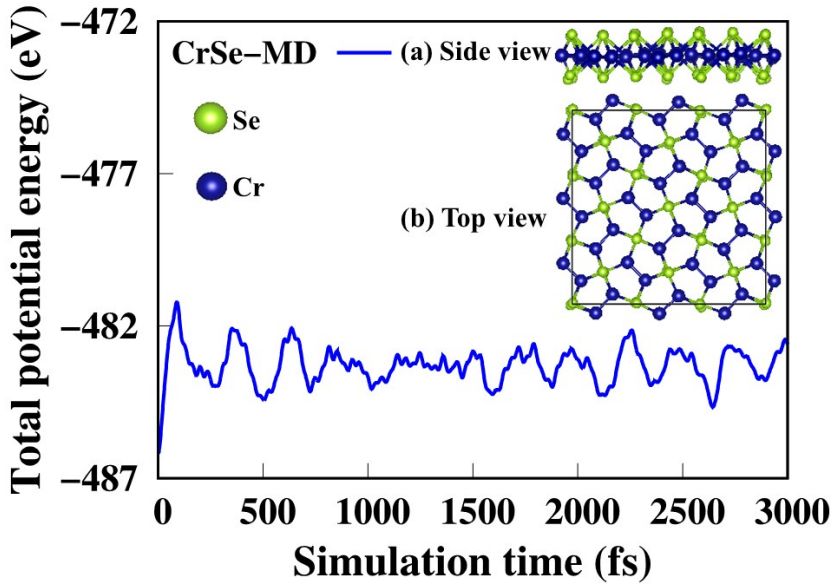

Figure S3. Total potential energy of penta-CrSe monolayer as a function of simulation time within canonical ensemble at a constant temperature of 300K. The insets are the (a) side and (b) top views of the configuration after 3 ps (3000 fs).

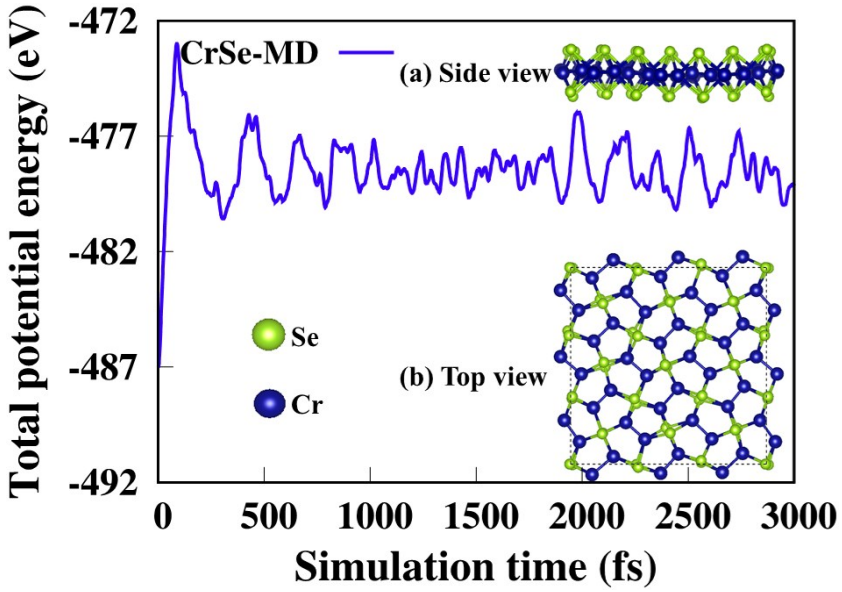

Figure S4. Total potential energy of penta-CrSe monolayer as a function of simulation time within canonical ensemble at a constant temperature of 800K. The insets are the (a) side and (b) top views of the configuration after 3 ps (3000 fs).

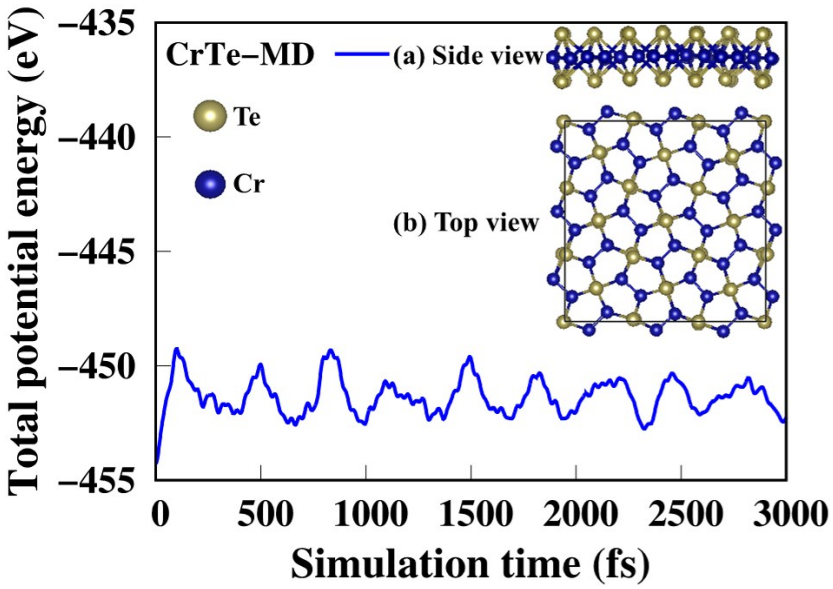

Figure S5. Total potential energy of penta-CrTe monolayer as a function of simulation time within canonical ensemble at a constant temperature of 300K. The insets are the (a) side and (b) top views of the configuration after 3 ps (3000 fs).

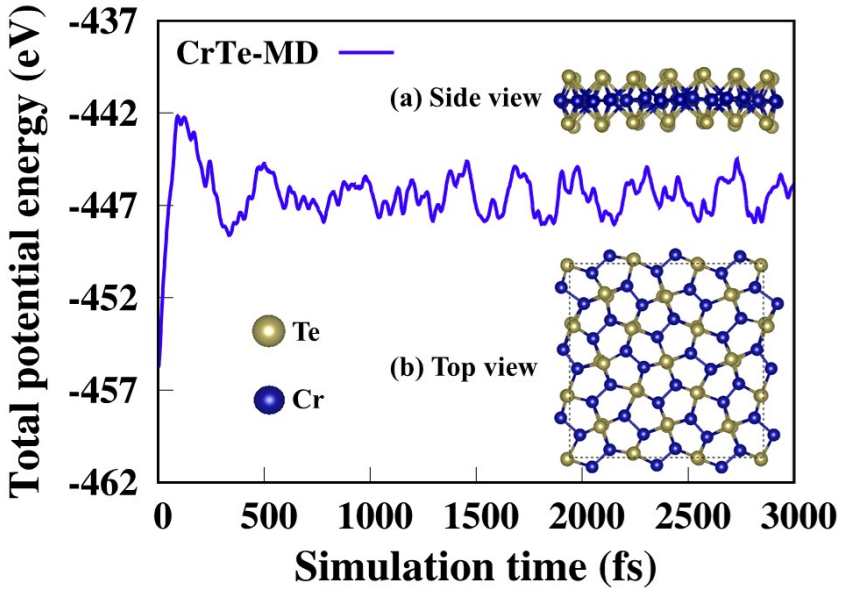

Figure S6. Total potential energy of penta-CrTe monolayer as a function of simulation time within canonical ensemble at a constant temperature of 800K. The insets are the (a) side and (b) top views of the configuration after 3 ps (3000 fs).

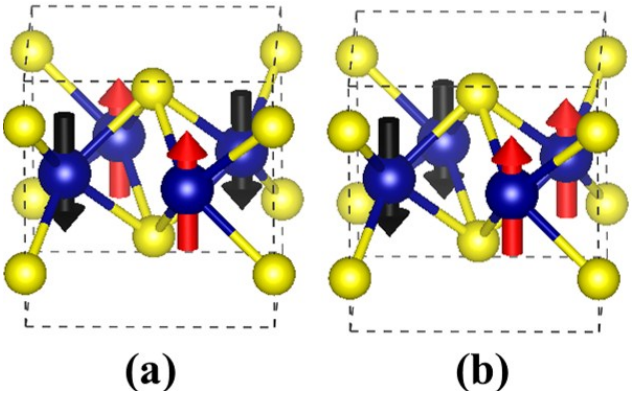

Figure S7 Antiferromagnetic (AFM) spin ordering using penta-CrS monolayer as representative: (a) AFM1 and (b) AFM2; Yellow and blue balls represent S, and Cr atoms, respectively; Red and black allows denote up and down directions of spins, respectively.

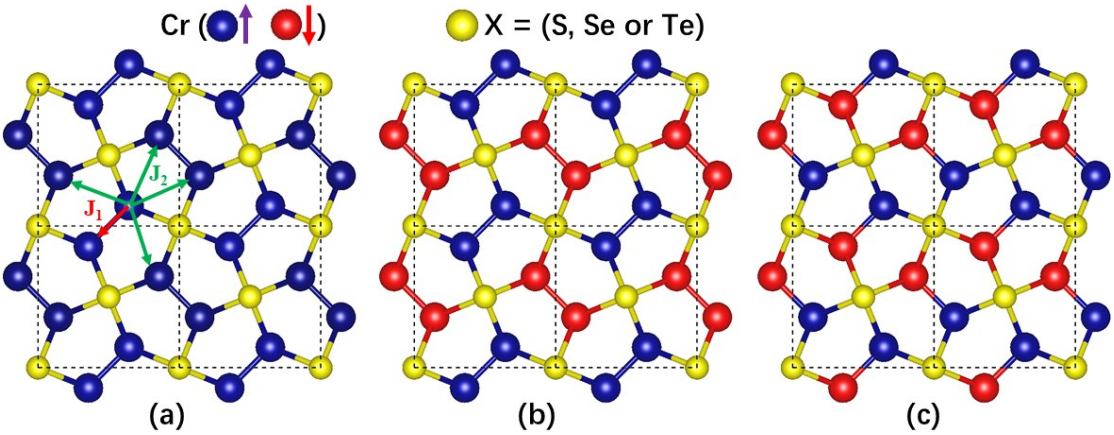

Figure S8 Nearest (J_1 marked in red) and next-nearest (J_2 marked in green) exchange interactions of the Ising model for (a) FM (b) AFM1 and (c) AFM2 states. Blue and red balls represent Cr atoms with up spin and down spin, while yellow balls are S, Se or Te atoms.