Supplementary information

Manipulating the electronic structure and physics properties in monolayer $Mo_2I_3Br_3$ via strain and doping

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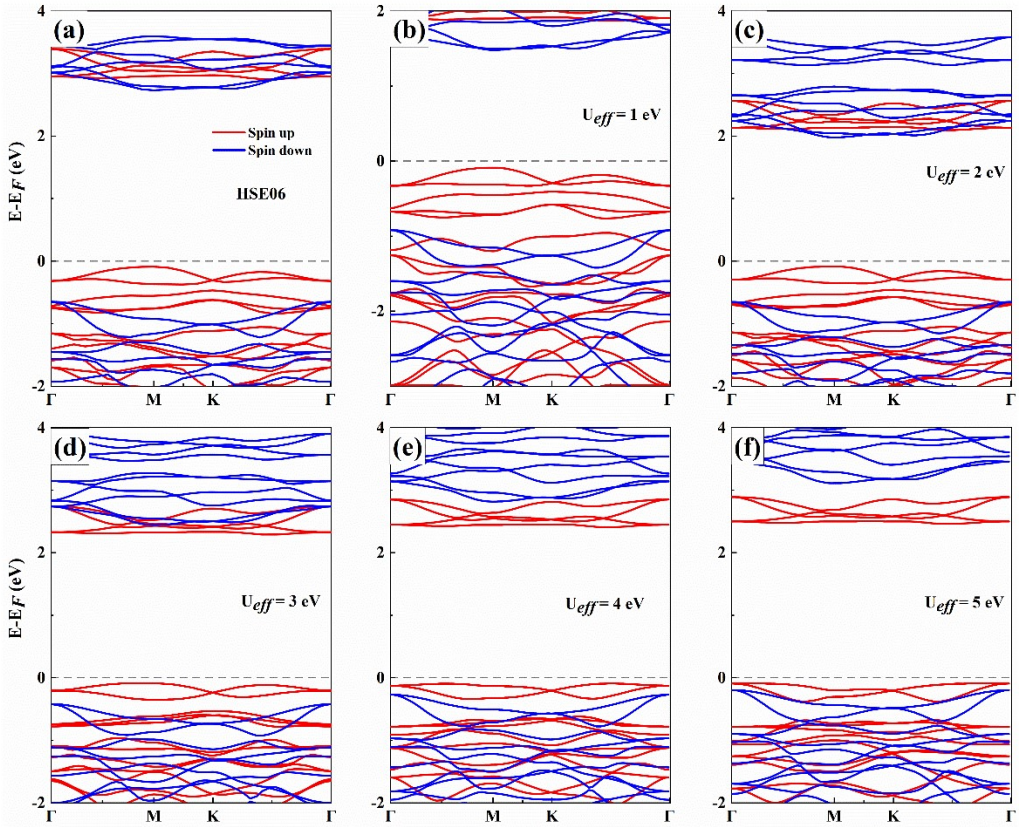

Figure. S1 The on-site Hubbard U_{eff} dependence of band structures. The gray horizontal dashed lines denote the Fermi level.

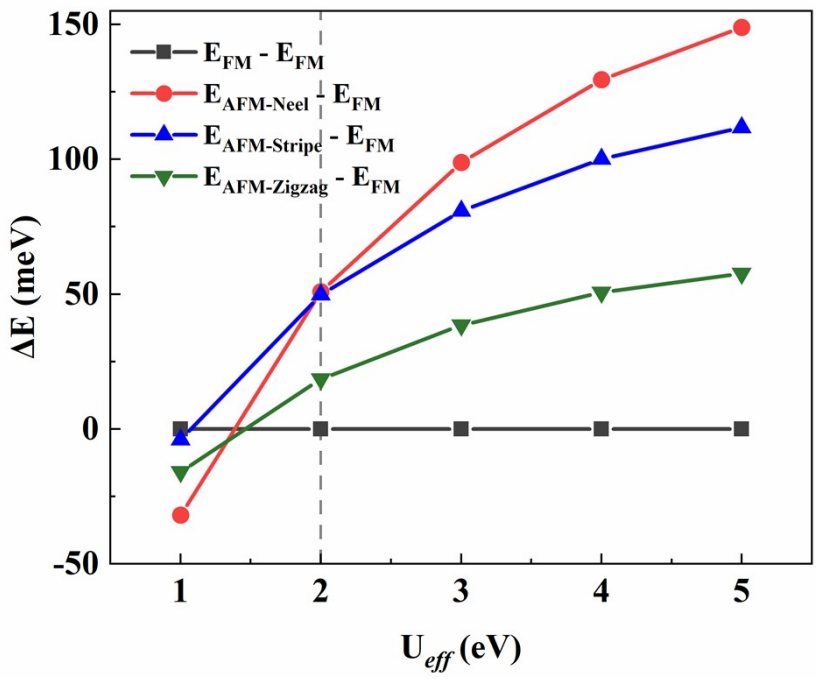

Figure. S2 The energy difference between different magnetic orderings as a function of on-site Hubbard U_{eff} in monolayer $Mo_2I_3Br_3$. We set U_{eff} = 2.0 eV in the calculation, corresponding to a ferromagnetic ground state.

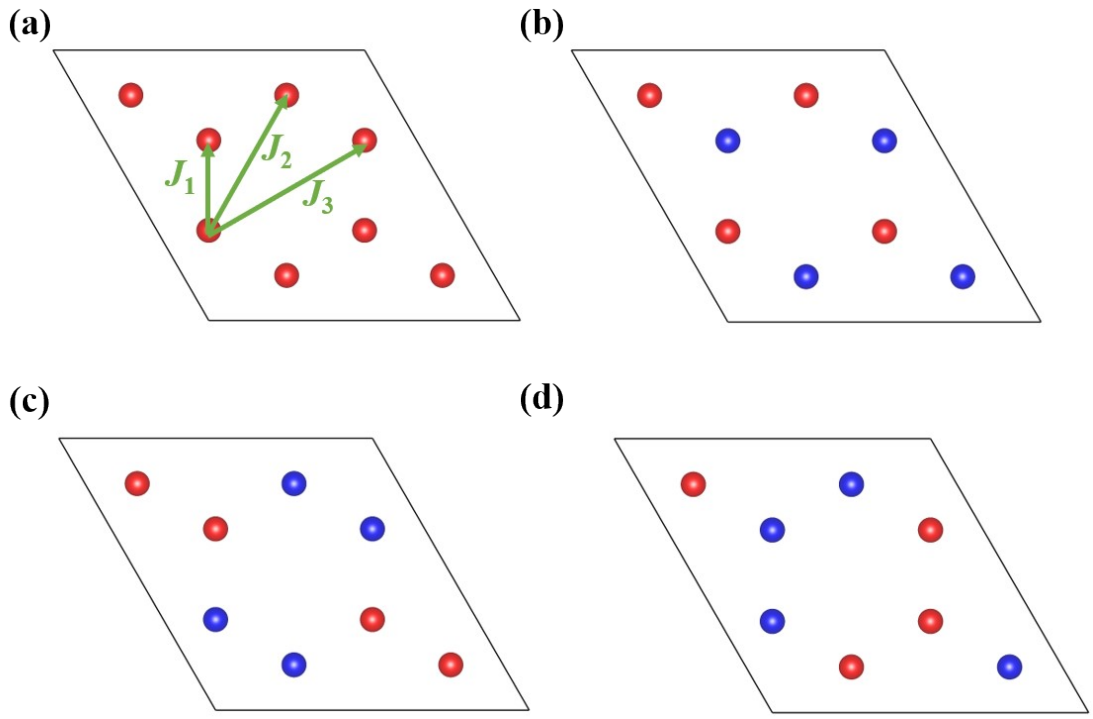

Figure. S3 The considered magnetic configurations of the monolayer $Mo_2I_3Br_3$: (a) FM, (b) Neel-

AFM, (c) Stripe-AFM, and (d) Zigzag-AFM. The green arrows denote the exchange paths.