Supplementary information for "Prediction of Half-Semiconductor Antiferromagnets with vanishing net Magnetization"

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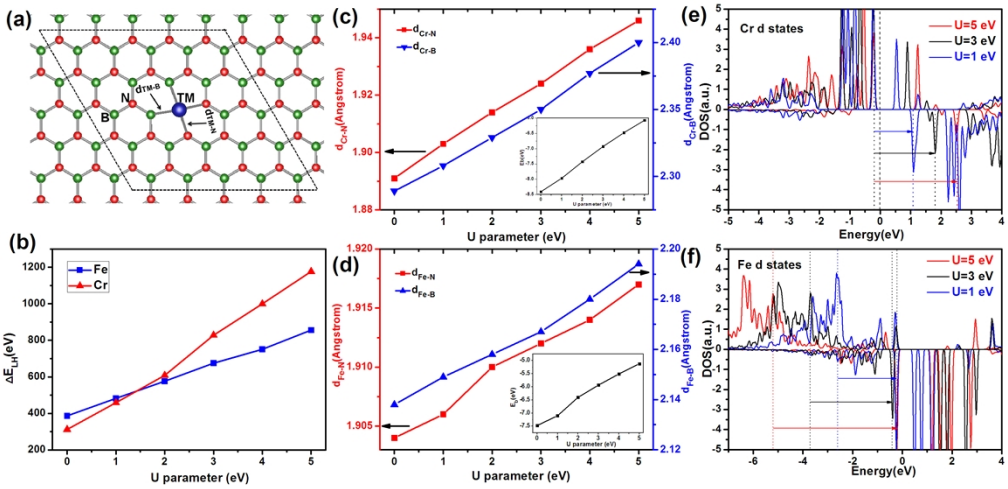

Figure S1 (a)The structure of single TM(Cr and Fe) doped BN sheet. (b) the energy difference between low spin states and high spin states for Cr and Fe, respectively with respect to U parameter. (c) and (d) represent the bond length(Fe-B, Fe-N, Cr-B and Cr-N) corresponding to the changing U parameter, where insert picture denoted the bind energy with U parameter for Cr and Fe, respectively. The PDOS for d states of Cr(e) and Fe (f) is in some typical U value.The Fermi level is set to zero.

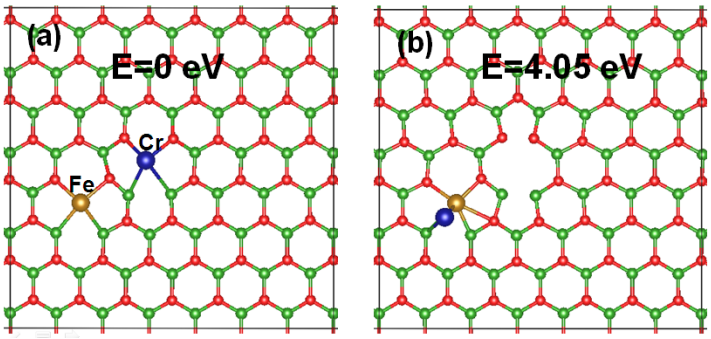

Figure S2 The compare energy between indirect (a) and direct (b) of Cr-Fe dimer. The reference energy for indirect case is set zero.