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Electronic Supplementary Information for

Induced half-metallic characteristic and enhanced magnetic anisotropy in two-dimensional Janus $V_2I_3Br_3$ monolayer by adsorbing graphyne

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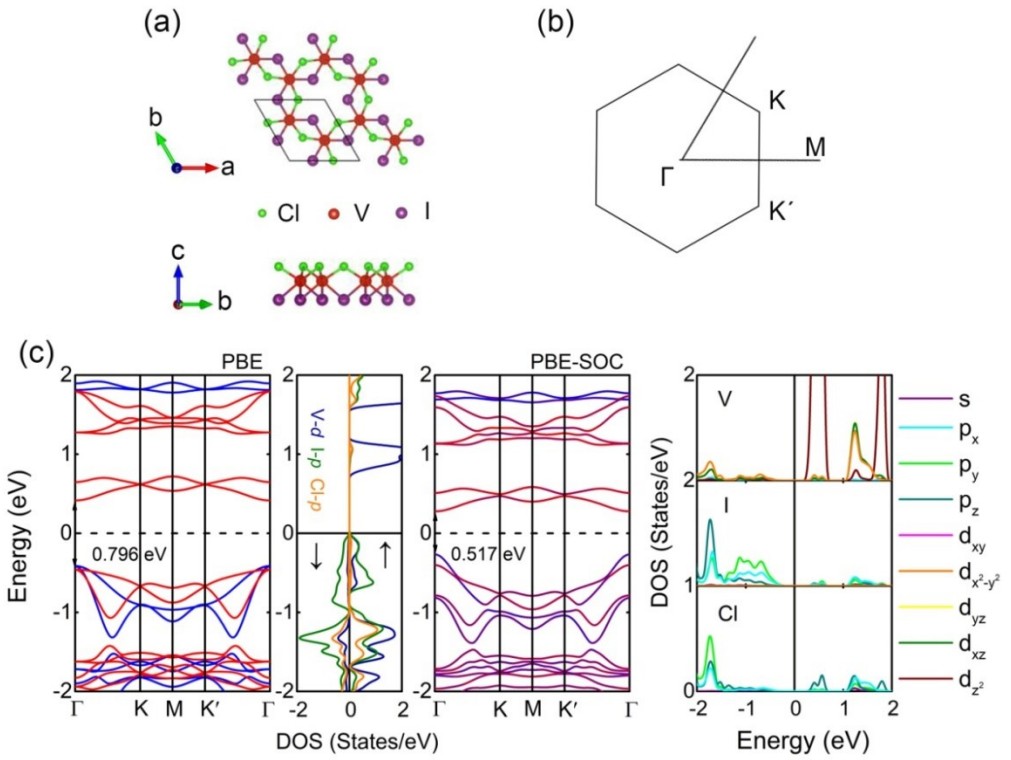

Fig. S1 (a) Crystal structure of Janus $V_2I_3Cl_3$ monolayer from the top and side views. (b) Hexagonal Brillouin zone. (c) Calculated band structure and PDOS of Janus $V_2I_3Cl_3$ monolayer. Red and blue lines represent the spin-up and spin-down channels. Fermi level is set to zero.

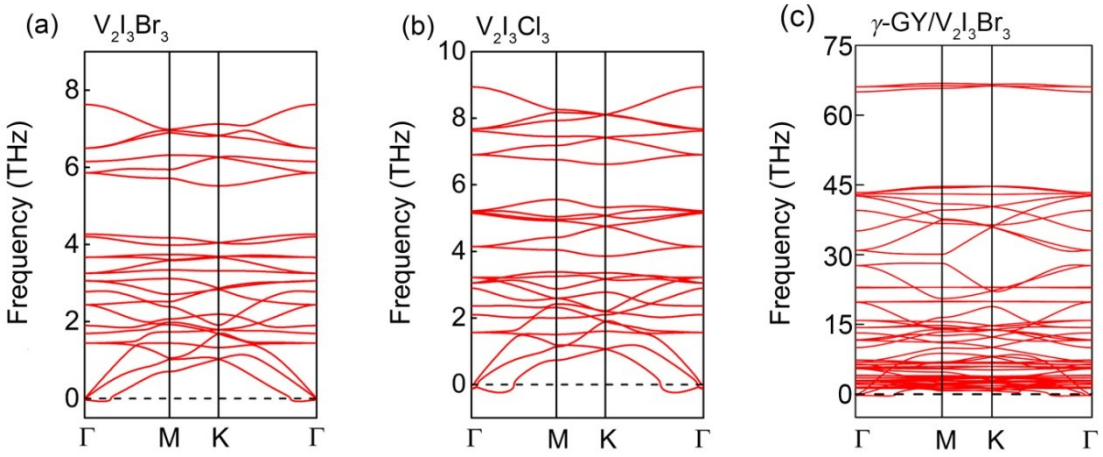

Fig. S2 Phonon spectrum of the Janus (a) $V_2I_3Br_3$, (b) $V_2I_3Cl_3$ monolayers and (c)the most stable γ-GY/$V_2I_3Br_3$ heterostructure.

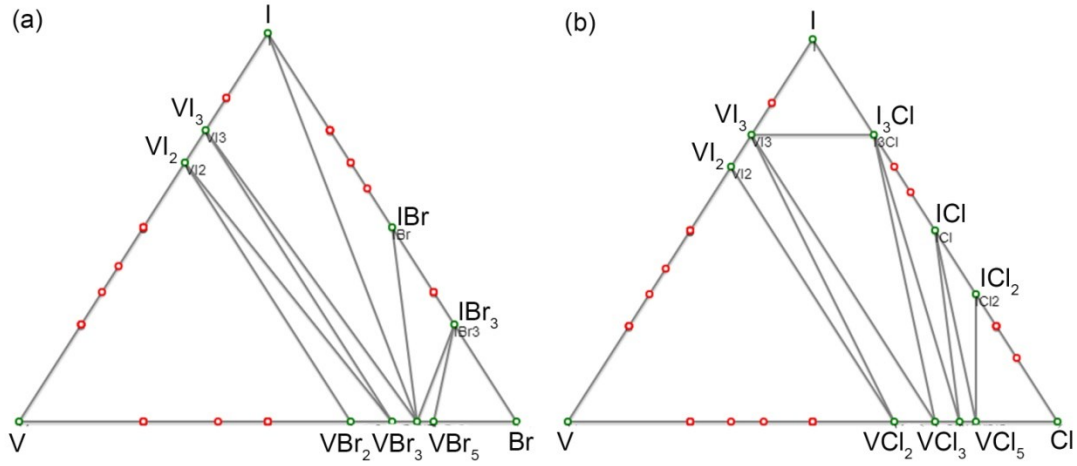

Fig. S3 Calculated phase diagrams of (a) Janus $V_2I_3Br_3$ and (b) $V_3I_3Cl_3$ monolayers.

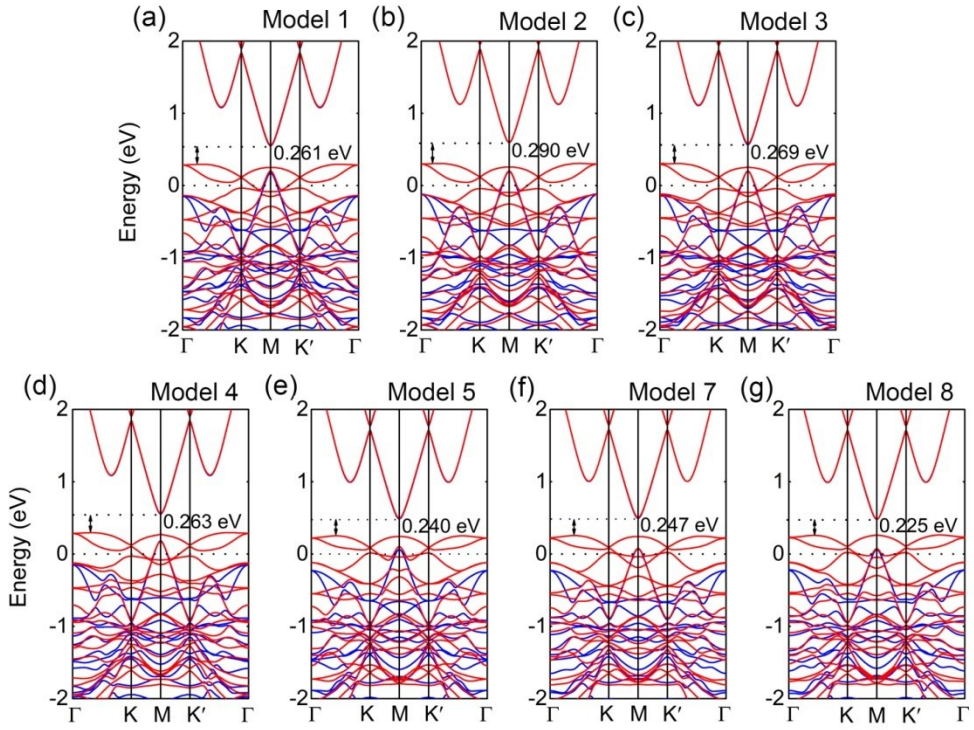

Fig. S4 (a)-(g) Band structure for γ-GY/$V_2I_3Br_3$ heterostructures of model 1-5 and model 7-8. Red and blue lines represent the spin-up and spin-down channels. Fermi level is set to zero.

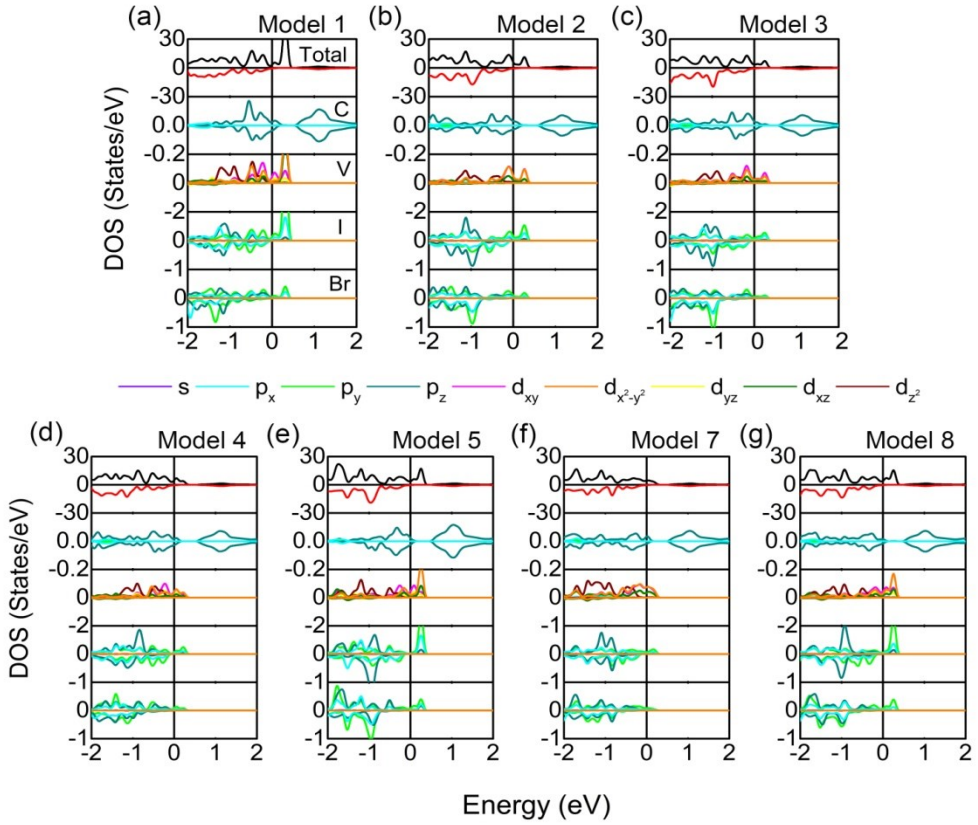

Fig. S5 (a)-(g) Spin-resolved total DOS and PDOS for γ-GY/$V_2I_3Br_3$ heterostructures of model 1-5 and model 7-8.

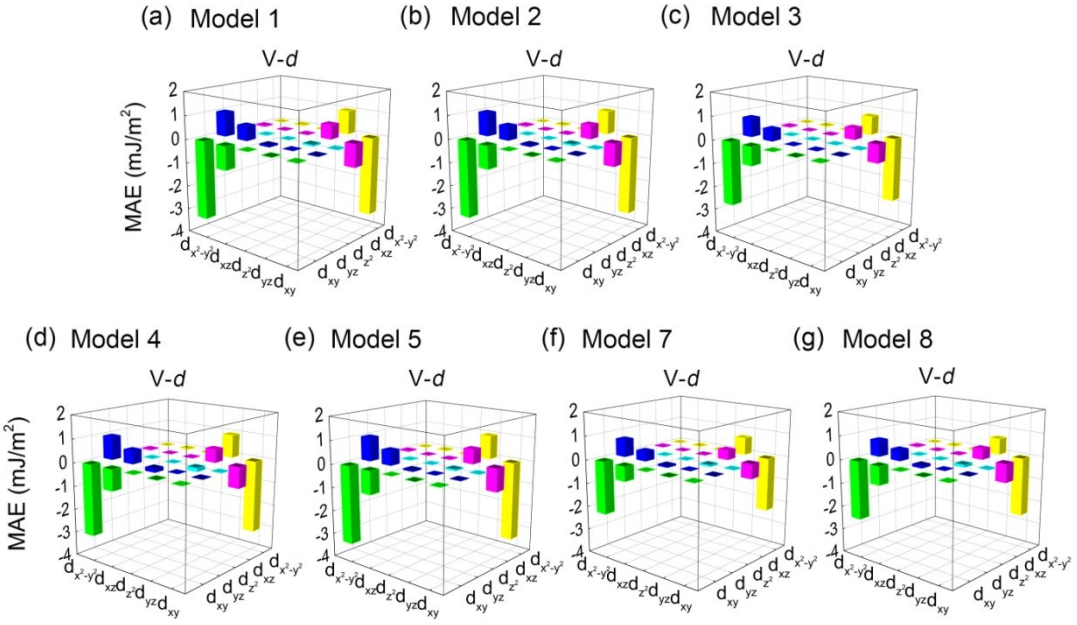

Fig. S6 (a)-(g) V-*d* orbital-resolved MAE in model 1-5 and model 7-8. The negative MAE from hybridization between V-*d* orbitals represents PMA.

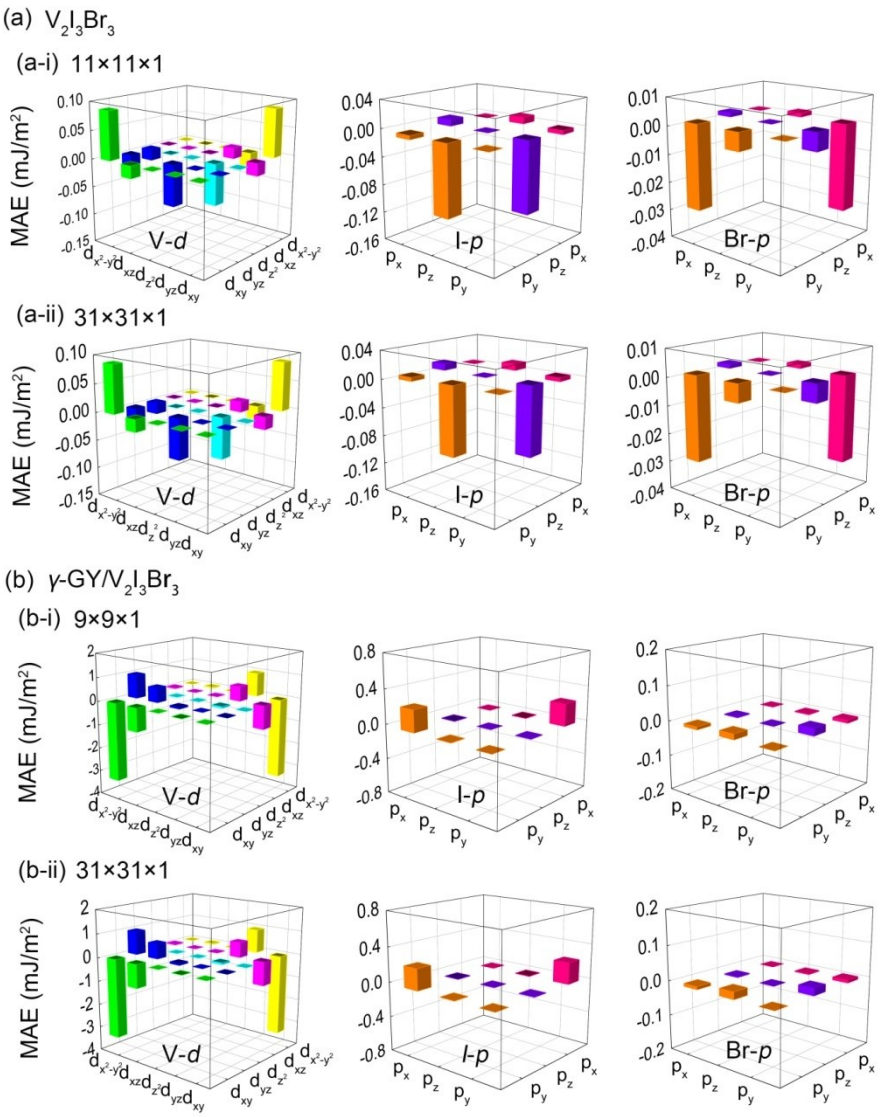

Fig. S7 Orbital-resolved MAE of V-*d*, I-*p* and Br-*p* orbitals in Janus $V_2I_3Br_3$ monolayer and *γ*-GY/$V_2I_3Br_3$ heterostructure at different k-point meshes.