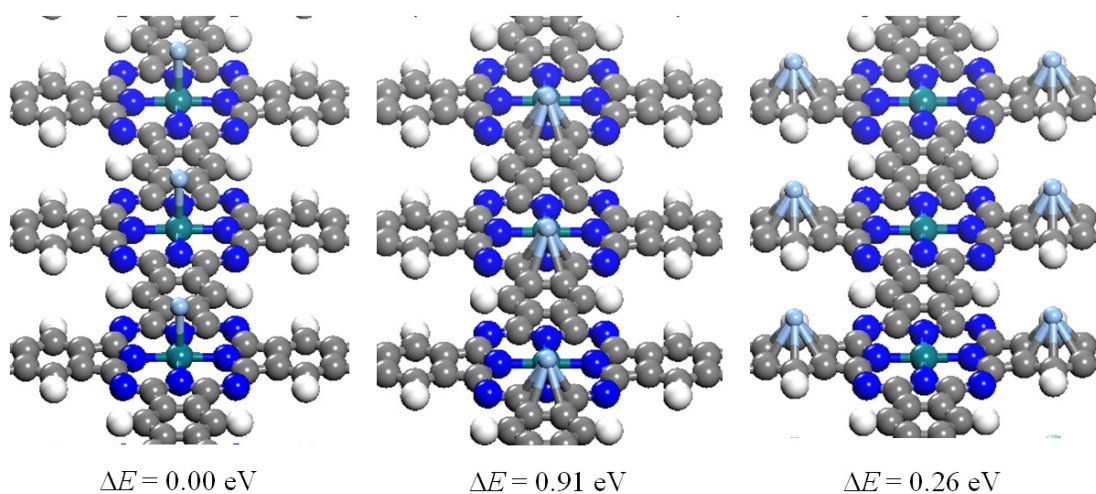


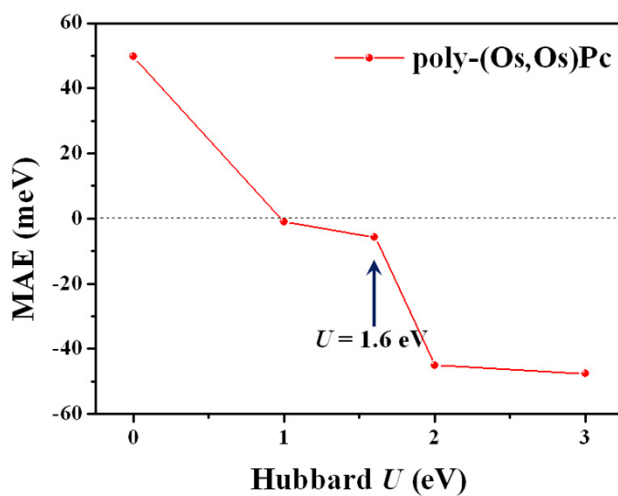
## Supporting Information

### Giant Magnetocrystalline Anisotropy of 5*d* Transition Metal-based Phthalocyanine Sheet

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**Figure S1.** Relative energies of the Ir atom adsorbed on Rh (left panel), on pentagon (middle panel), and on hexagon of poly-(Ir,Rh)Pc (right panel).



**Figure S2.** Magnetic anisotropy energy of poly-(Os,Os)Pc as a function of Hubbard  $U$  on Os.