

## Supplementary Information

### Giant Magnetic Moments of B and C doped Cuboctahedral $Mn_{13}$ Clusters

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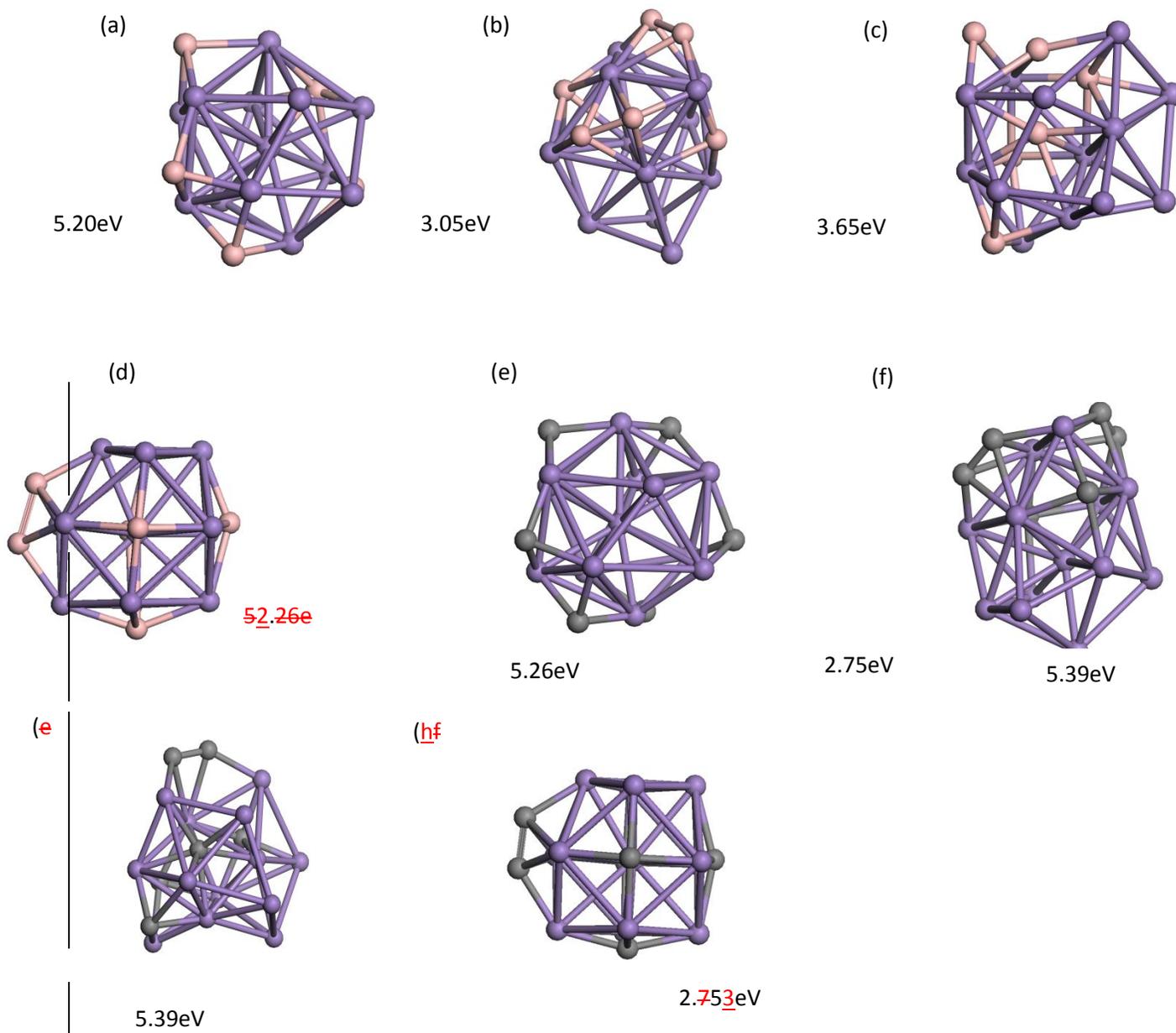


Figure S1 Relative energy of some other isomers of (a-cd) $\text{Mn}_{13}\text{B}_6$  and (de-fh) $\text{Mn}_{13}\text{C}_6$  referred to the ground-state cuboctahedral structures, ~~which (a-c, e-g)~~ are based on Ih structures doped by B or C at various locations. In (a)(d) dopants are allocated on surface separately, in (b)(e) they are grouped around the surface, and in (c)(f) one dopant atom is allocated in the center. In (d)(h) one dopant and one Mn atom swap positions in ground-state cuboctahedral structures.

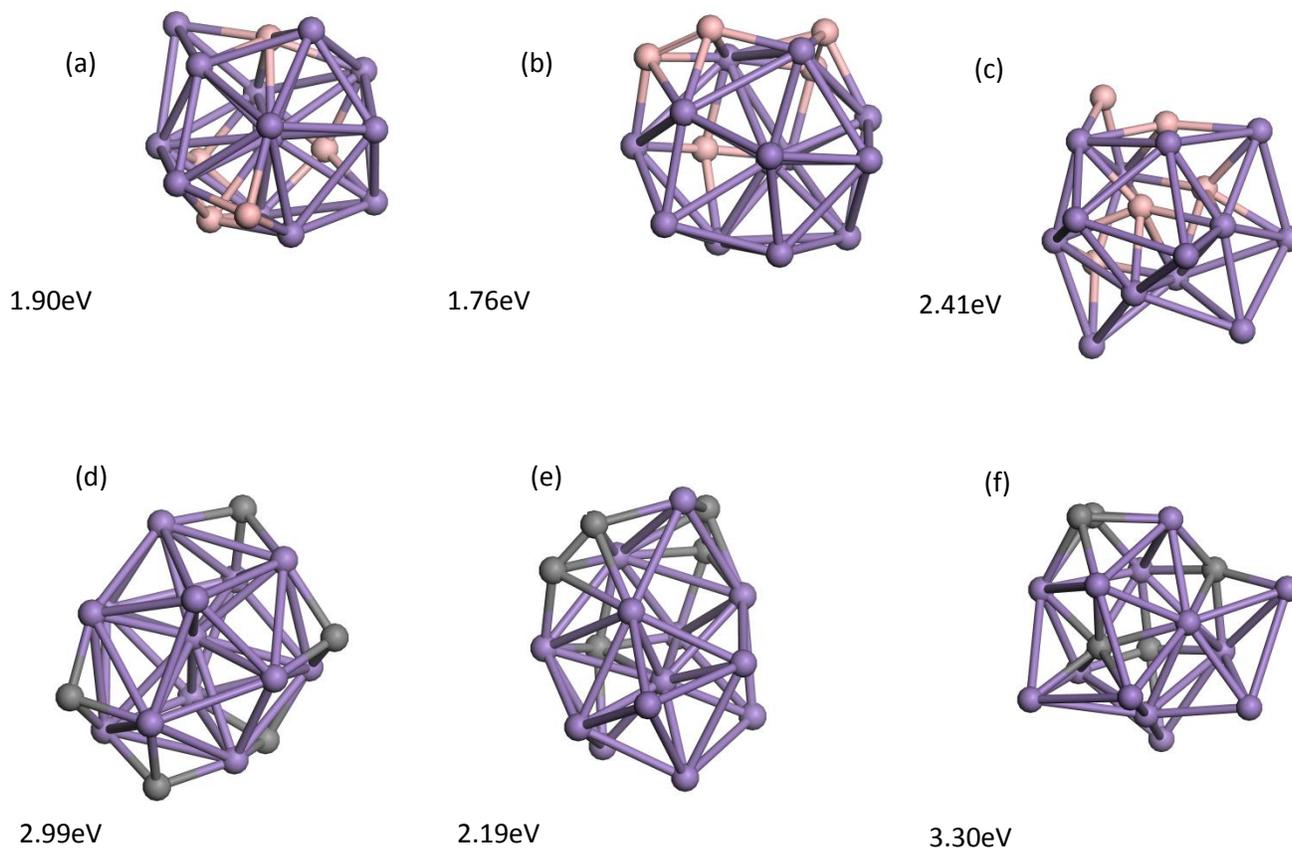


Figure S2 Relative energy of some other isomers of (a-c) $\text{Mn}_{13}\text{B}_5$  and (d-f) $\text{Mn}_{13}\text{C}_5$  referred to the ground-state respective cuboctahedral structures, which are based on Ih structures doped by B or C at various

locations. In (a)(d) dopants are allocated on surface separately , in (b)(e) they are grouped on the surface, and in (c)(f) one dopant atom is allocated in the center.