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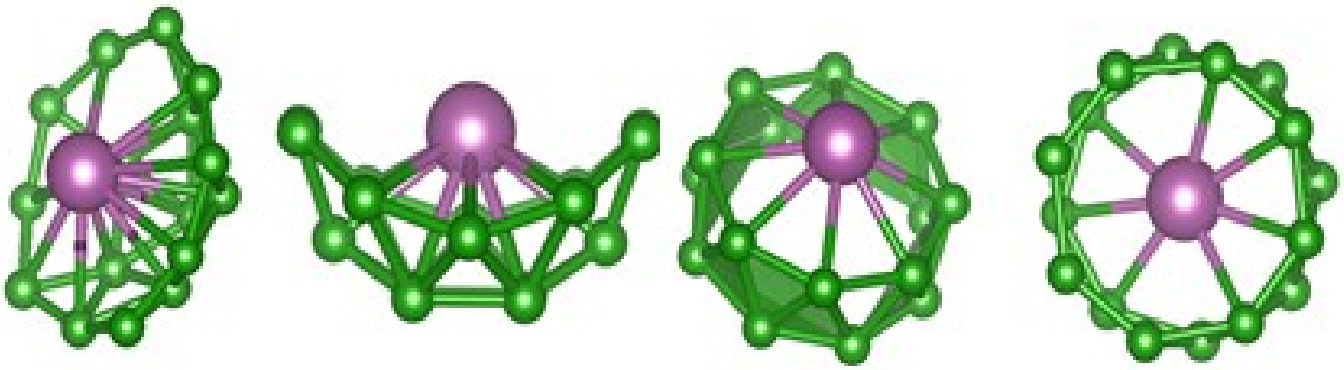
Supplementary Information for:

Evolutionary Search for $(M©B_{16})^{Q}$ (M=Sc-Ni; Q=0/-1) Clusters: Bowl/Boat- vs Tubular-Shape

Zabihollah Mahdavifar*, Fazel Shojaei

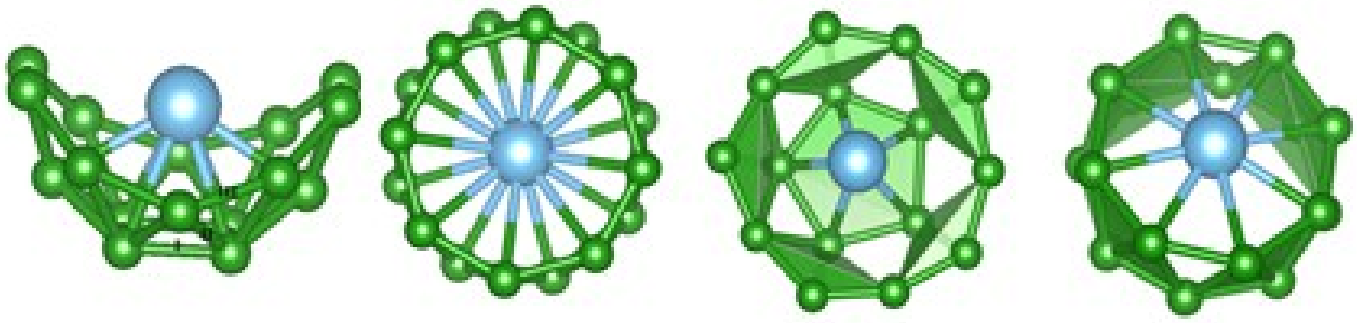
Department of Chemistry, Faculty of Science, Shahid Chamran University of Ahvaz, Ahvaz, Iran

Sc



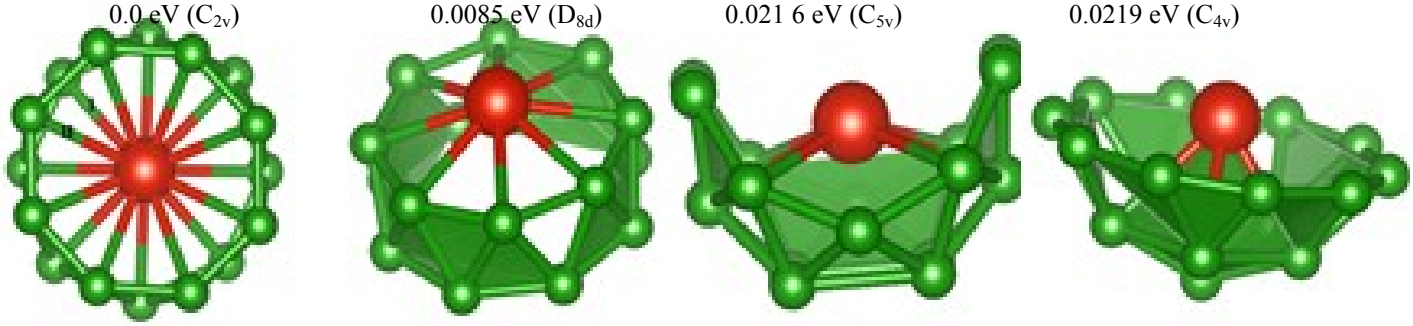
0.0 eV (C_{5v}) 0.021 eV (C_{2v}) 0.091 eV (C_{8v}) 0.186 eV (D_{8d})

Ti



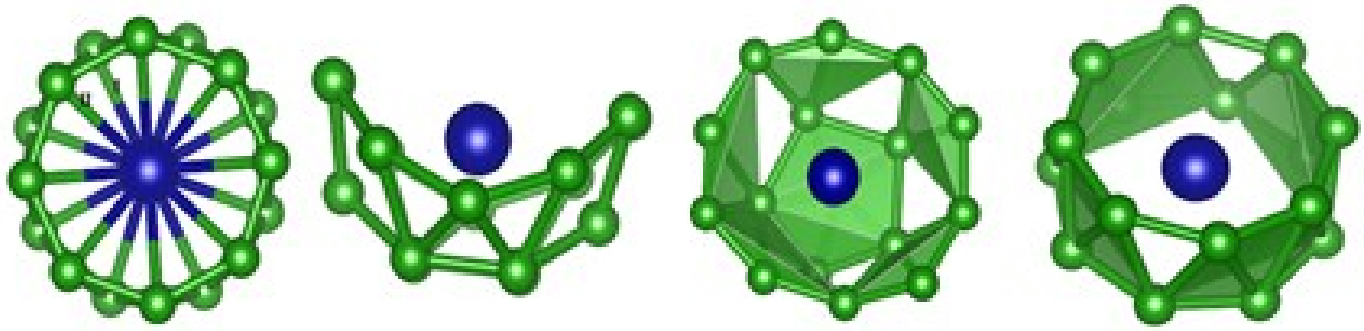
0.0 eV (C_{2v}) 0.0085 eV (D_{8d}) 0.021 6 eV (C_{5v}) 0.0219 eV (C_{4v})

V



0.0 eV (C_{2v}) 0.1025 eV (C_{8v}) 0.1034 eV (C_{2v}) 0.0994 eV (C_{5v})

Cr



0.0 eV (C_{2v}) 0.0675 eV (C_{2v}) 0.09090 eV (C_{5v}) 0.1059 eV (C_{4v})

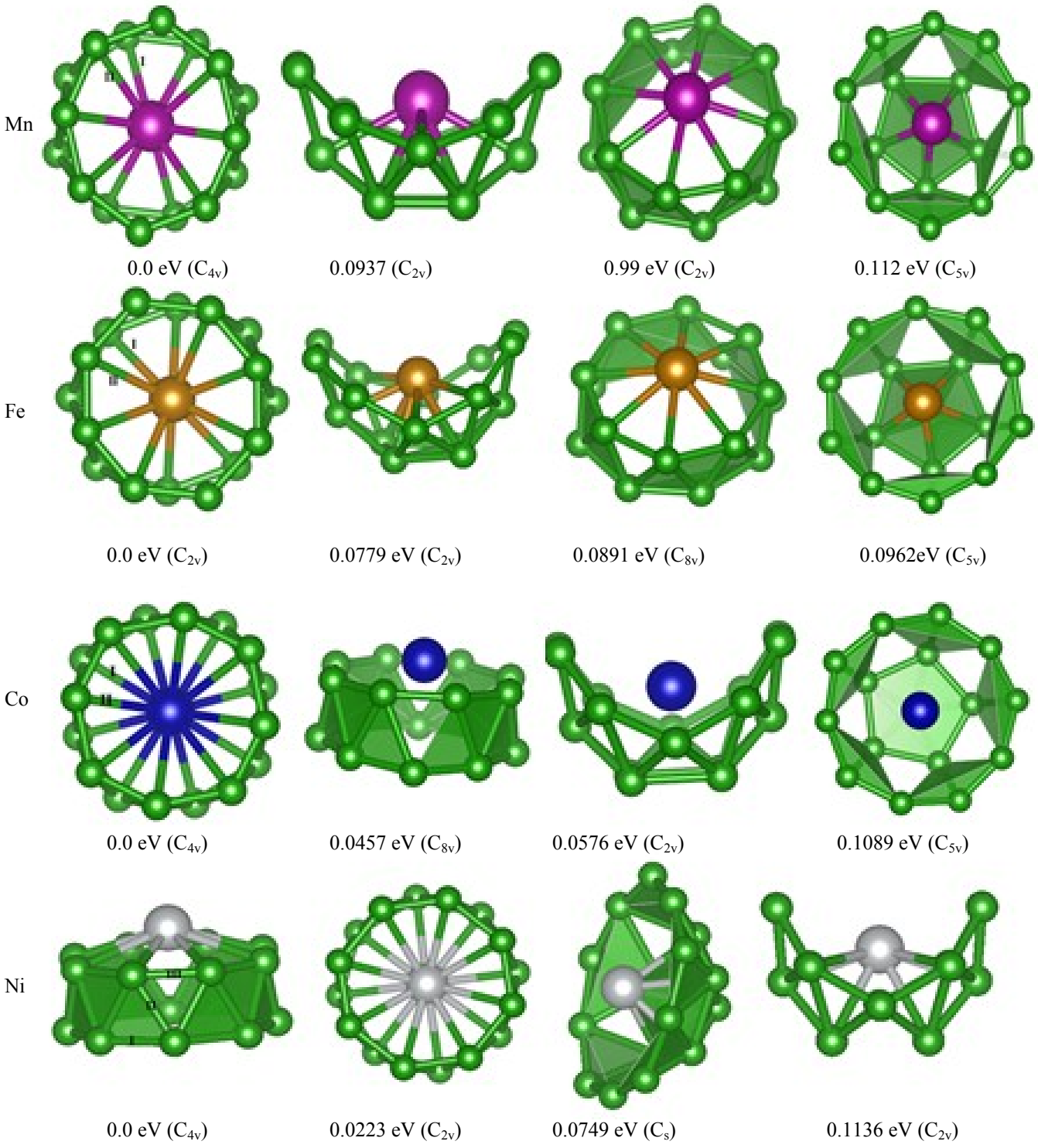
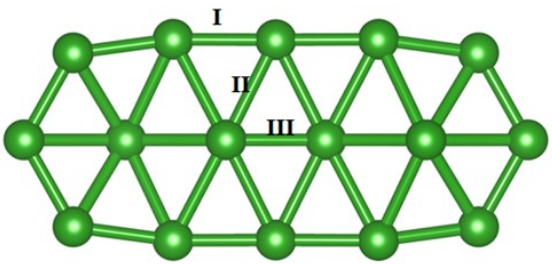
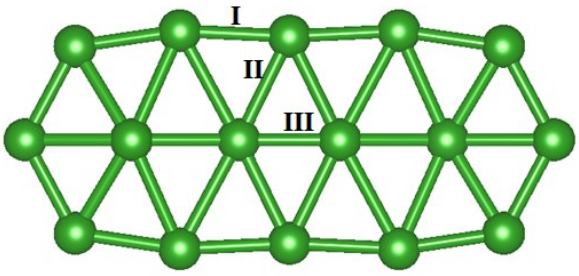


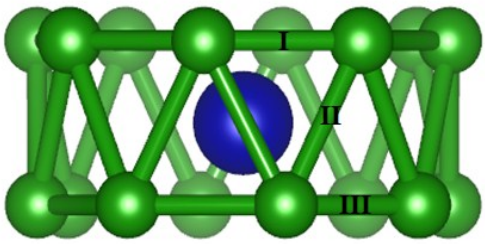
Figure S1: The most stable structure with some low-laying isomers of $(M©B_{16})^{-1}$ species. The wheel–shaped (M atom located on the center of tubular B_{16} species) for the M= V, Cr, Mn, Fe, Co is the lowest-energy. For Ni metal atom, the drum-shaped, where the M atom located out of the tubular B_{16} motif is the most stable structure; For the Sc and Ti the bowl and boat structures are the most stable structure, respectively. In the case of Cr, the drum shaped after re-optimization converted to the wheel shaped.

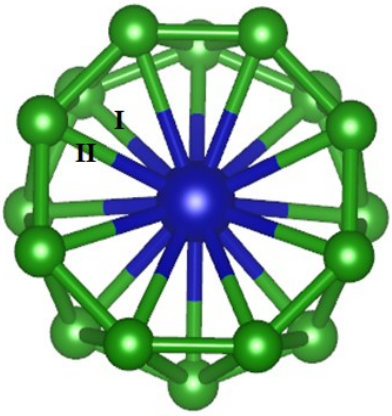


$(B_{16})^0$

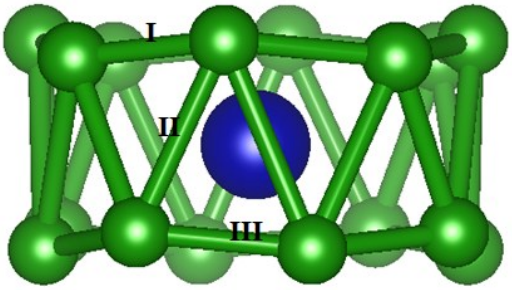


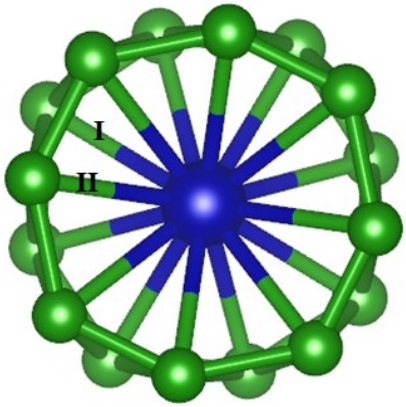
$(B_{16})^{-1}$



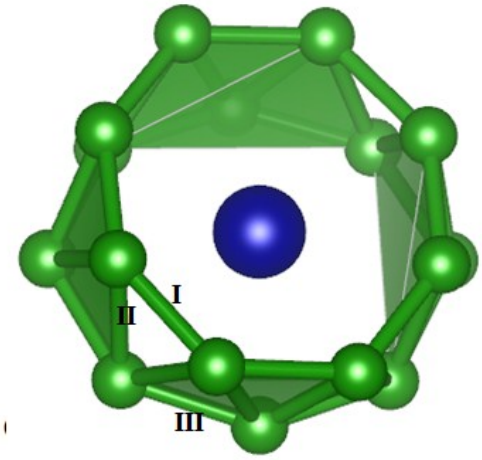


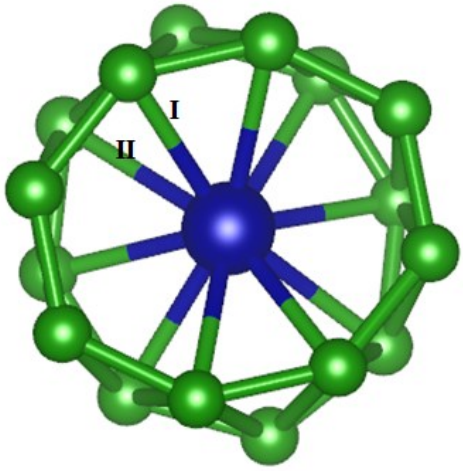
$(in\text{-}Co©B_{16})^0$





$in\text{-}(Co©B_{16})^{-1}$





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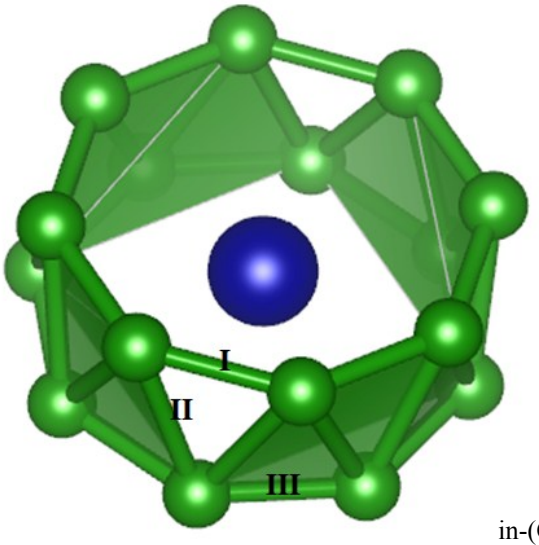
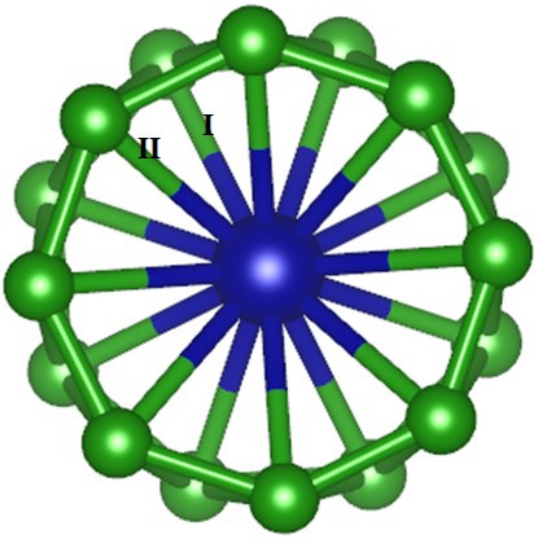
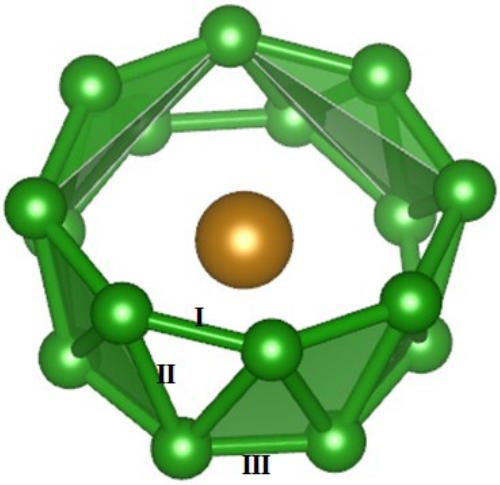
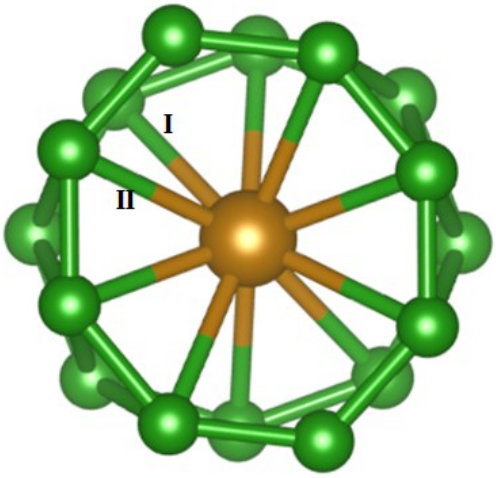


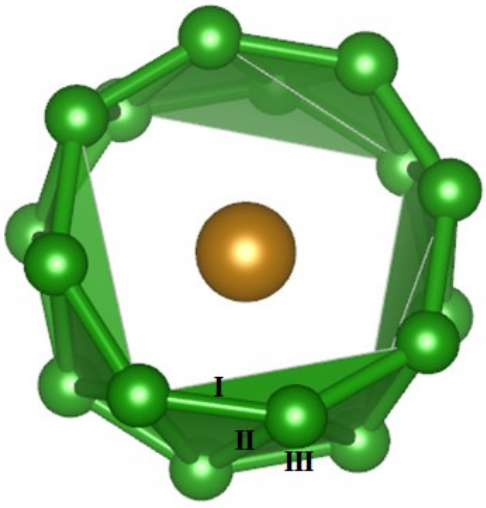


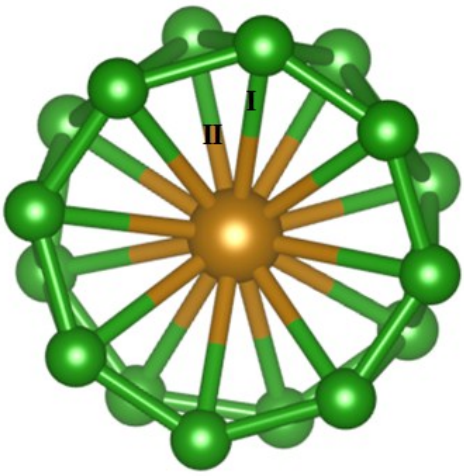
in-$(Cr©B_{16})^{-1}$





in-$(Fe©B_{16})^{0}$





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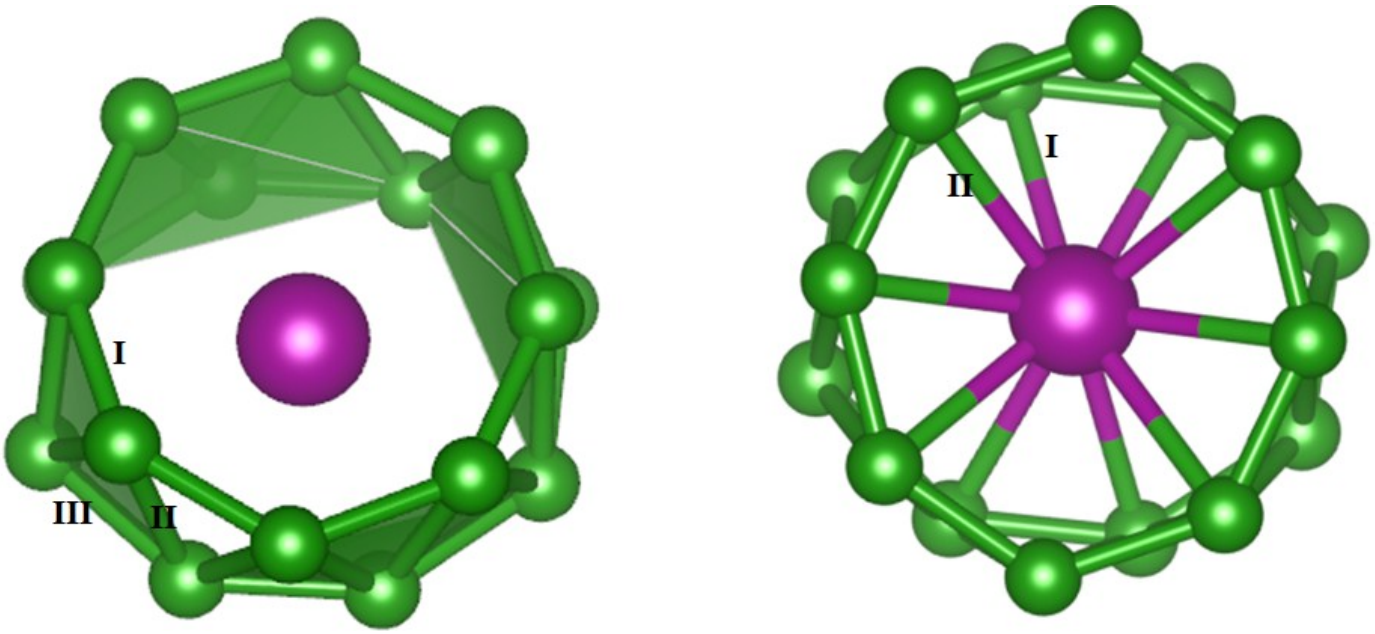
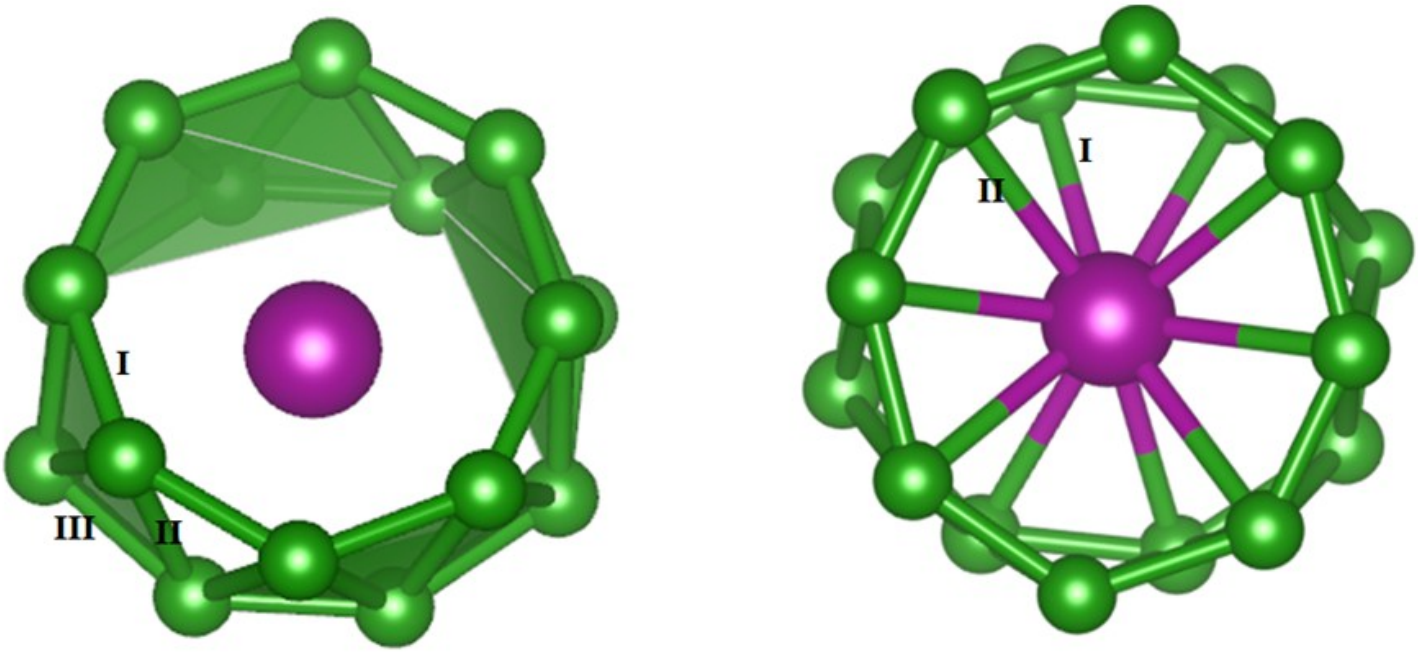


$(in\text{-}Mn©B_{16})^{0}$



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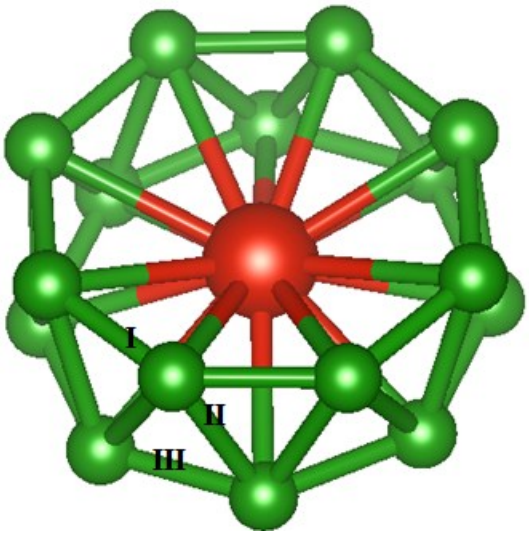
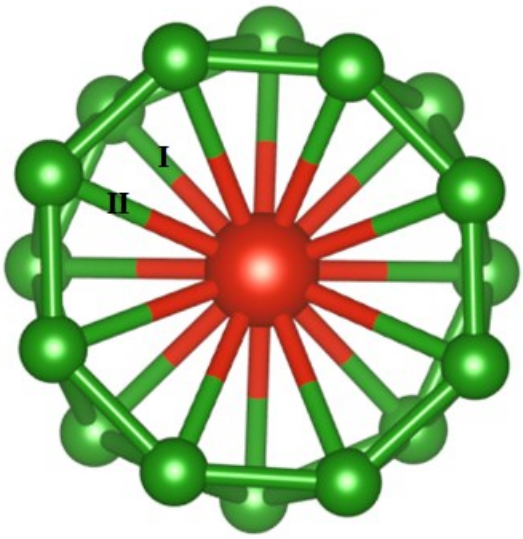
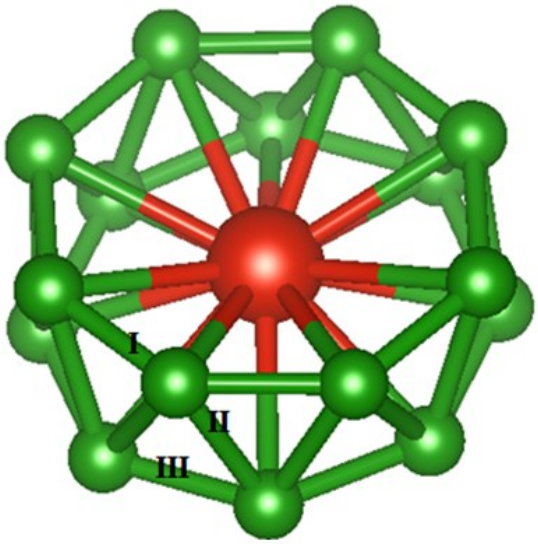
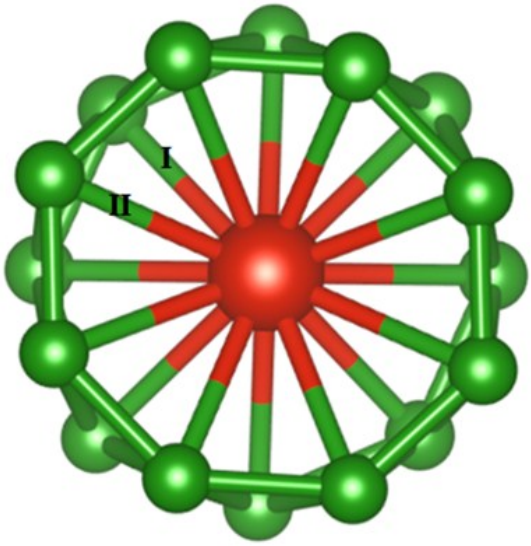


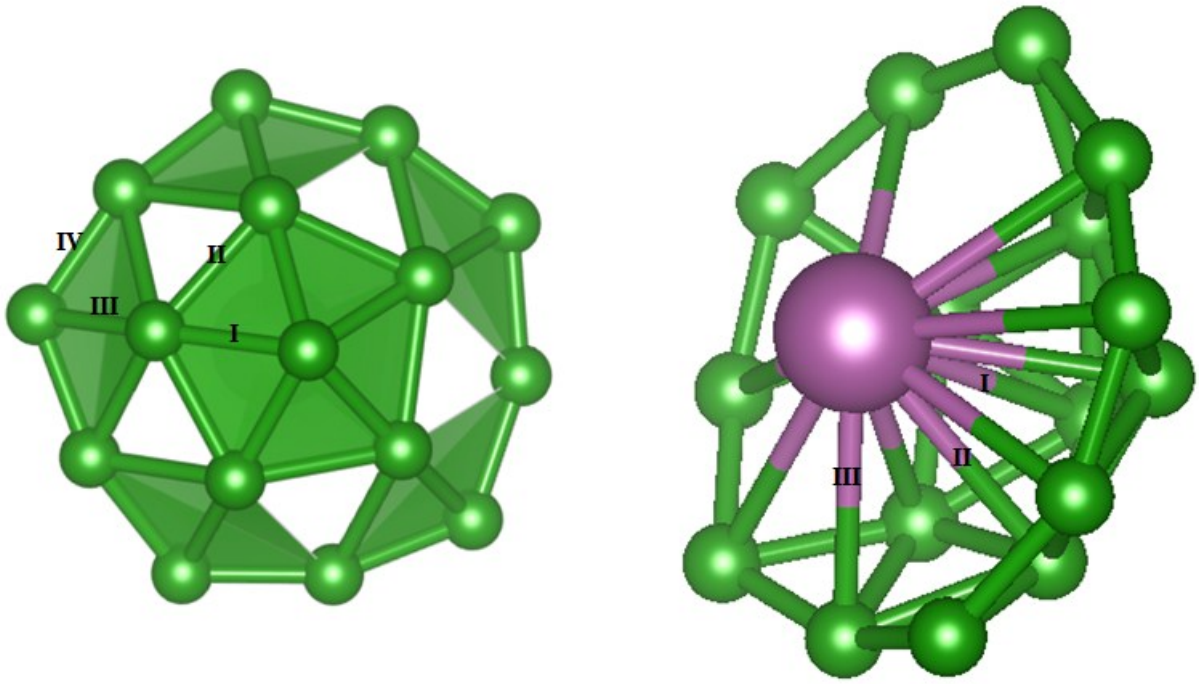


in-$(V©B_{16})^{0}$

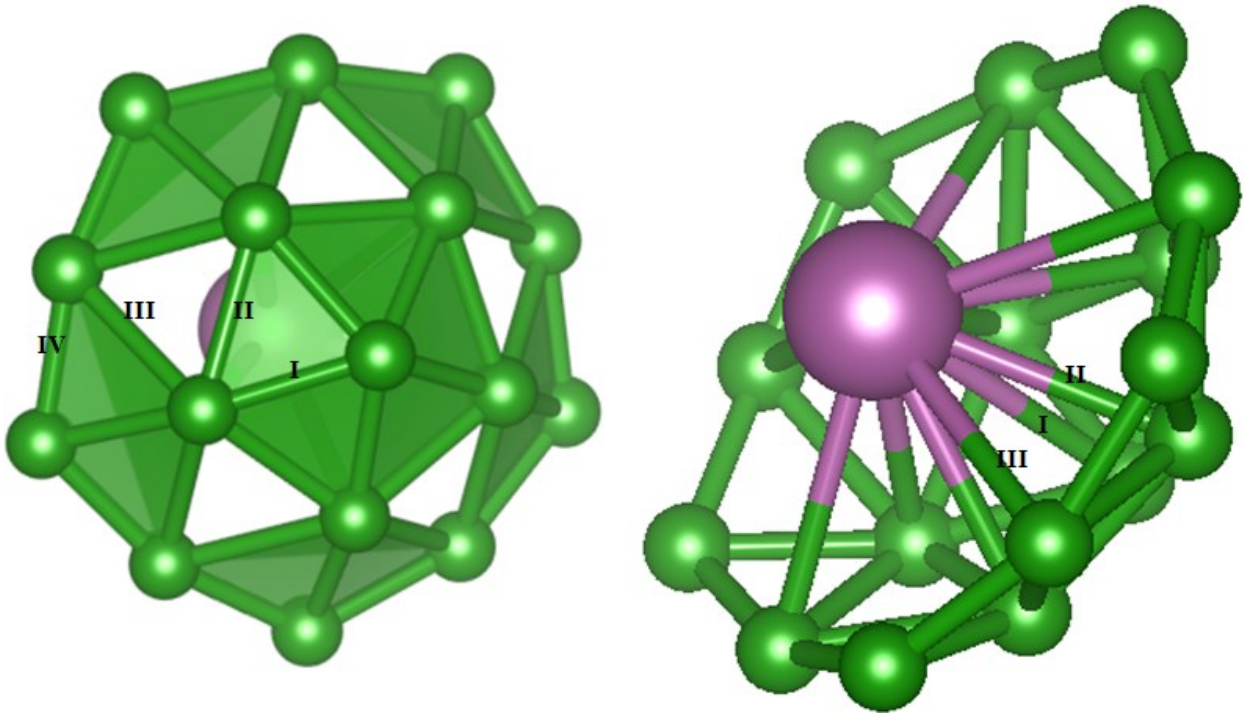




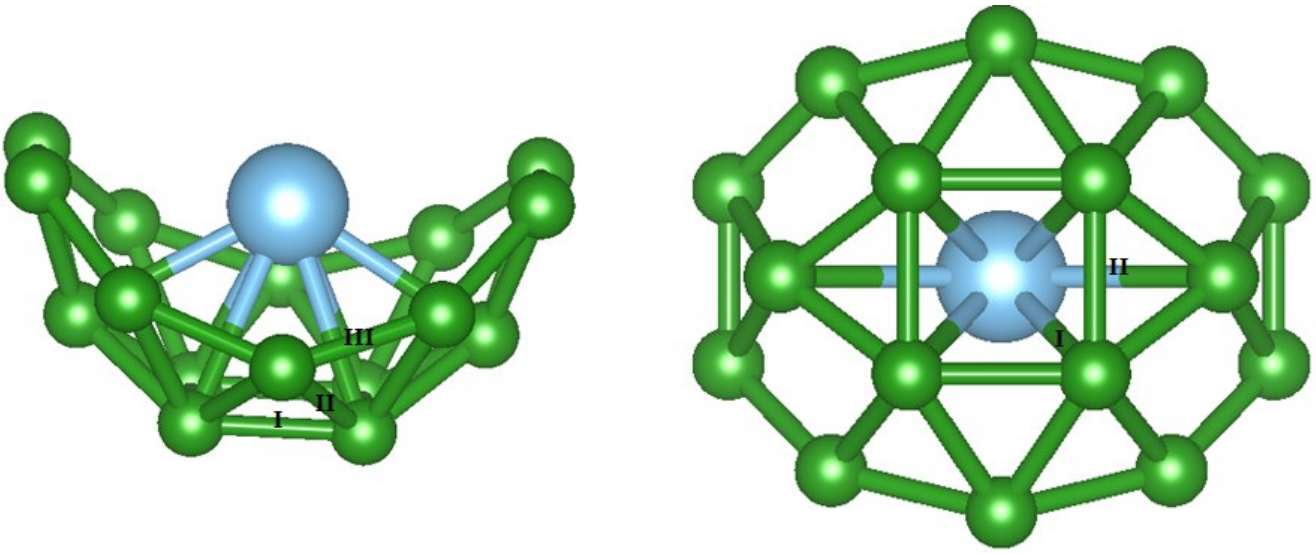
(in-$V©B_{16})^{-1}$



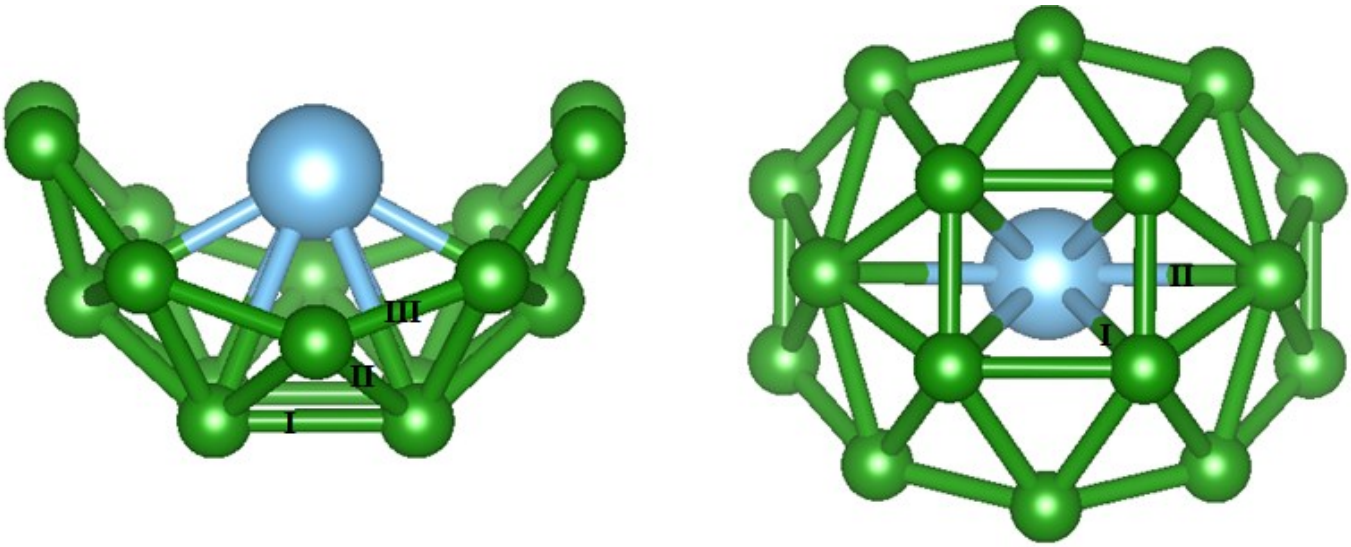
$(bowl\text{-}Sc©B_{16})^{0}$



$bowl\text{-}(Sc©B_{16})^{-1}$



$(boat\text{-}Ti©B_{16})^{0}$



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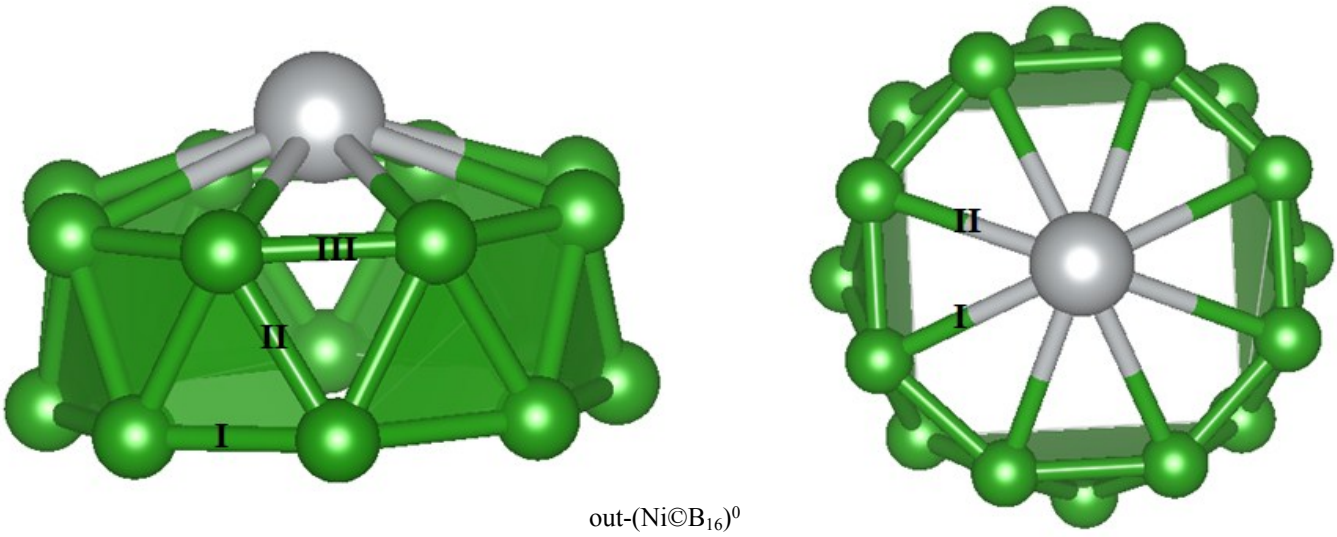
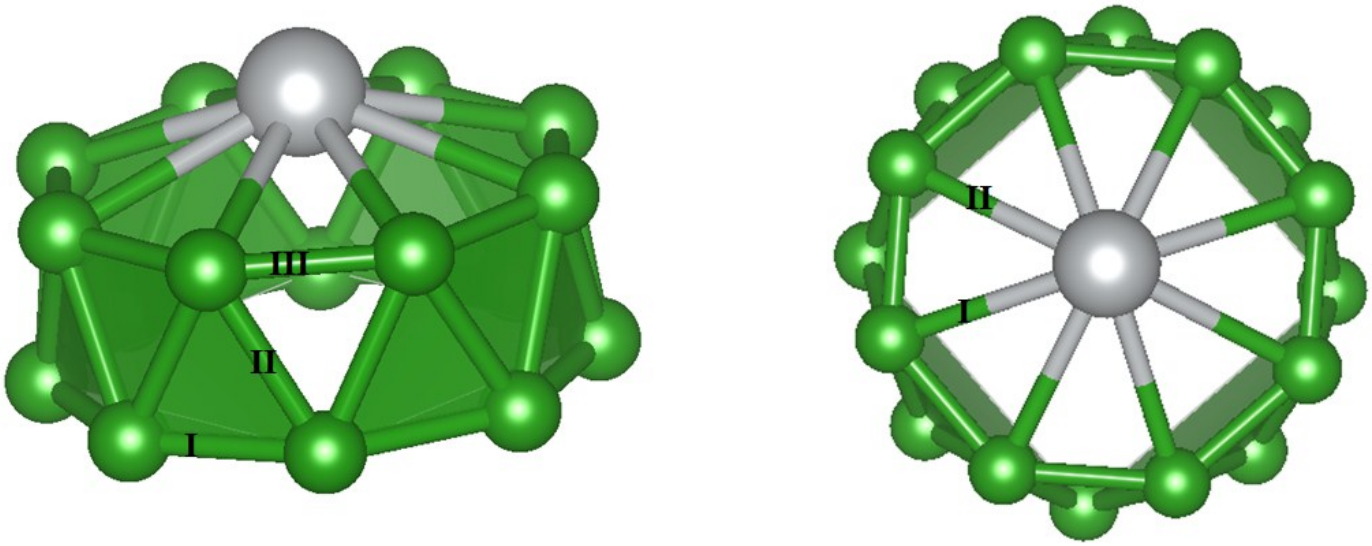
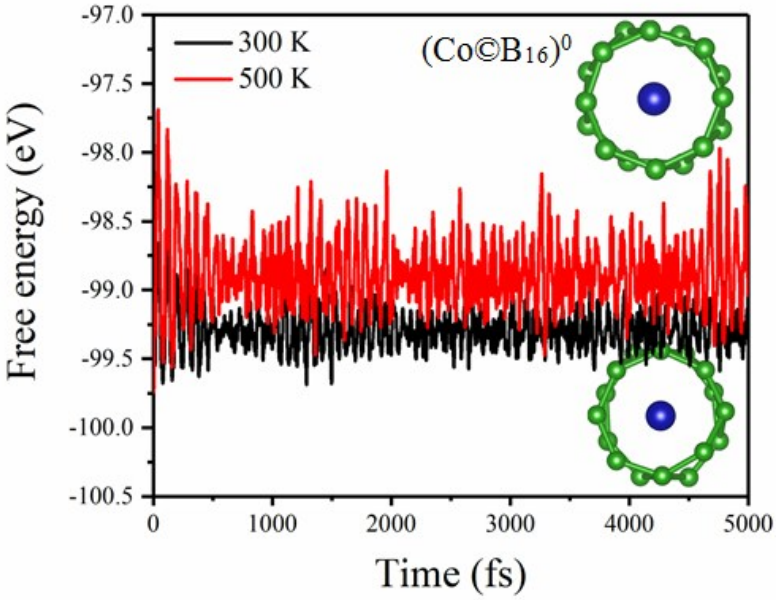


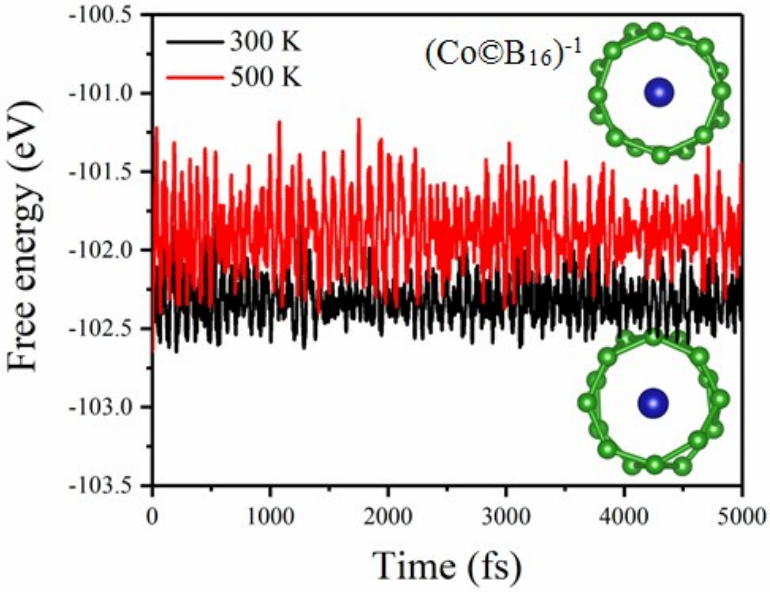
out-$(Ni©B_{16})^0$

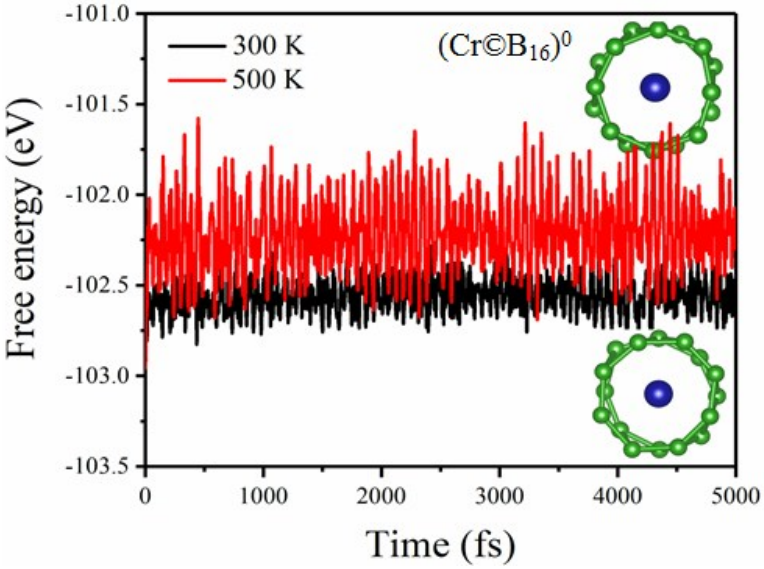


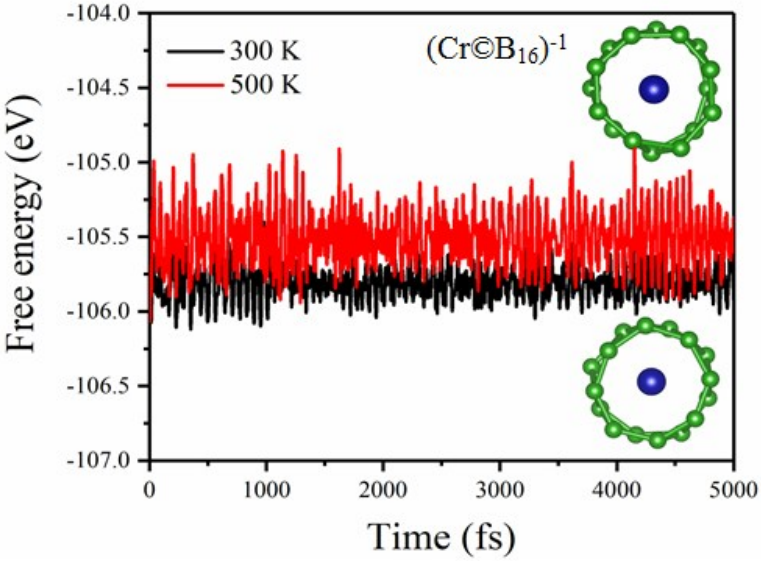
$(out\text{-}Ni©B_{16})^{-1}$

Figure S2: Relaxed geometry of the most stable structure of $(B_{16})^Q$ and $(M©B_{16})^Q$ clusters obtained at HSE06 level of theory.


300 K
500 K
(Co©B16)0
Free energy (eV)
Time (fs)


300 K
500 K
(Co©B16)-1
Free energy (eV)
Time (fs)


300 K
500 K
(Cr©B16)0
Free energy (eV)
Time (fs)


300 K
500 K
(Cr©B16)-1
Free energy (eV)
Time (fs)

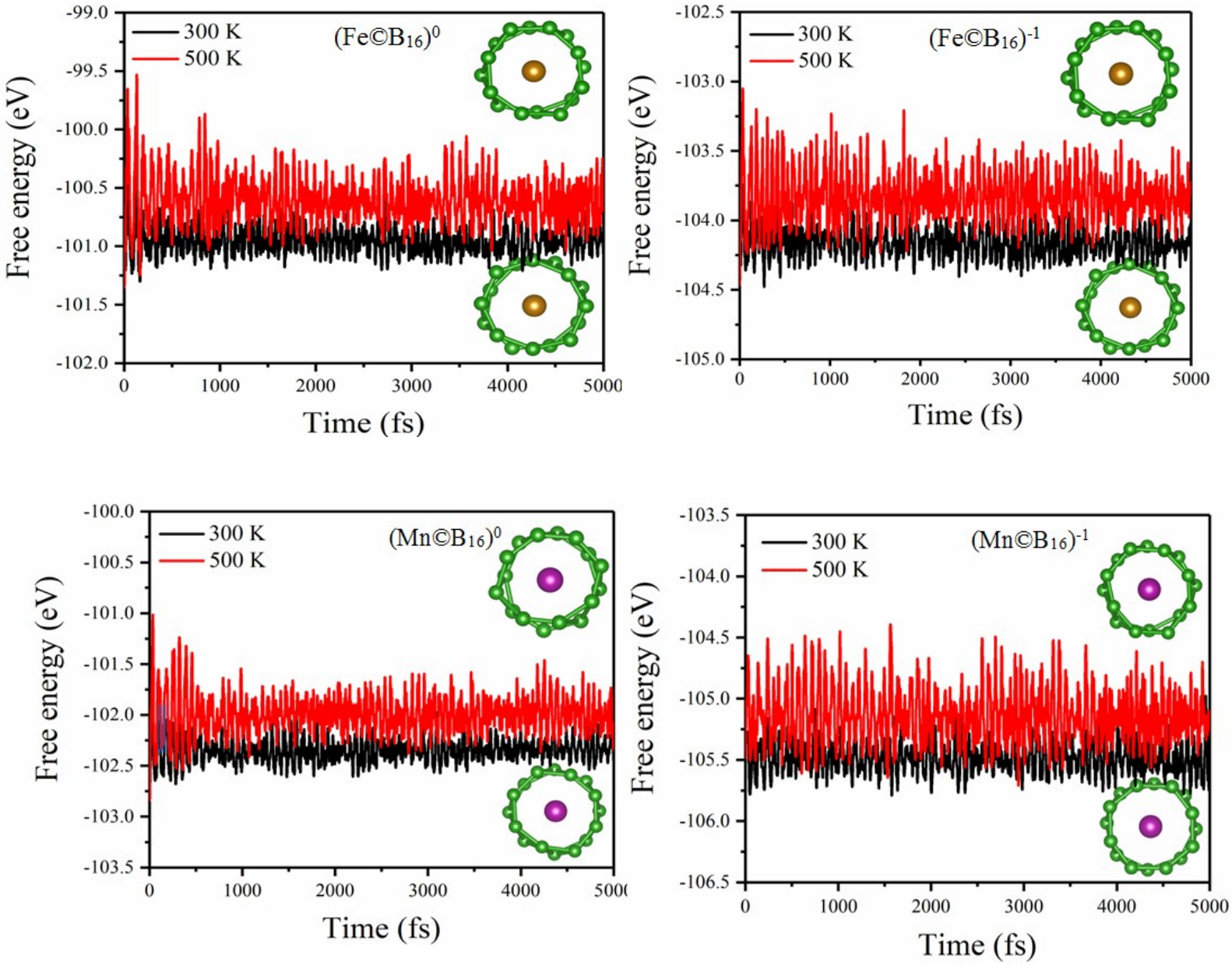
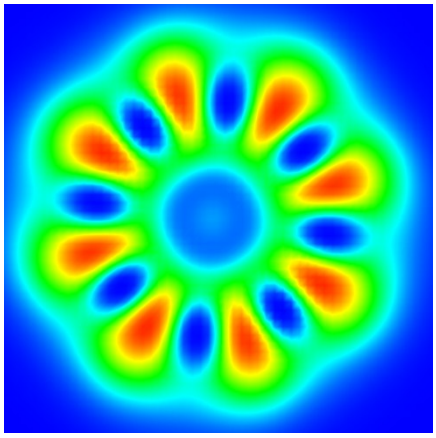
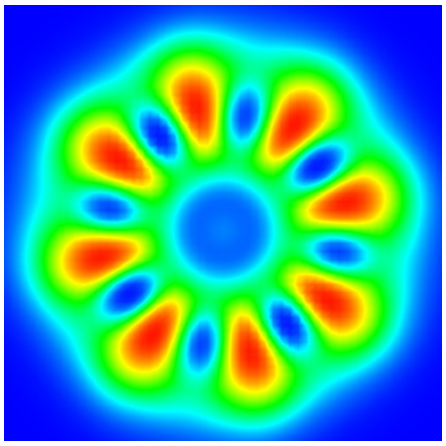


Figure S3: The snapshots of the most stable structures for a time of 5 ps. The temperature of the AIMD was set to 300 and 500 K.

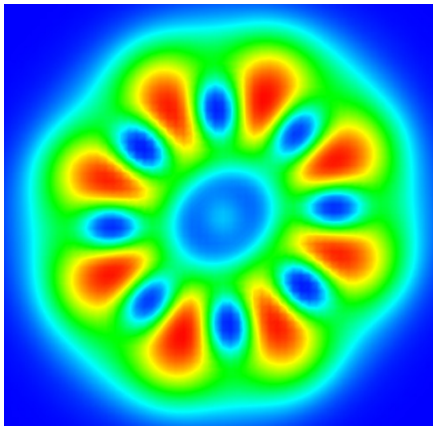
negative

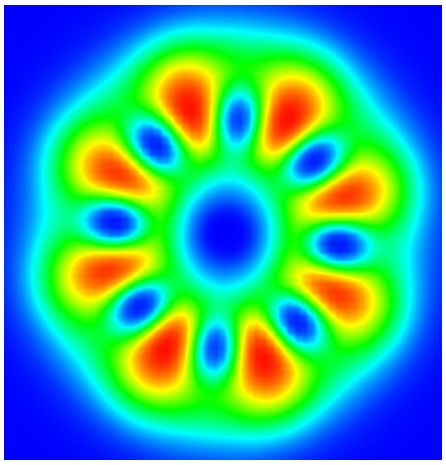


neutral

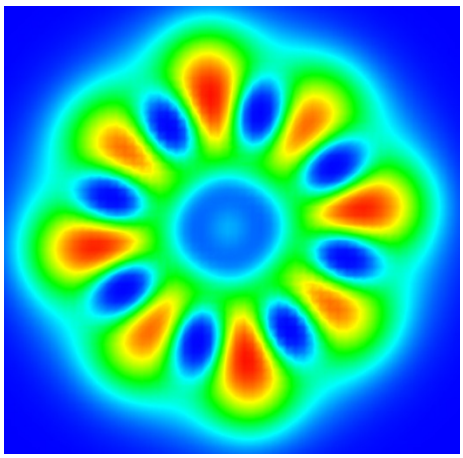


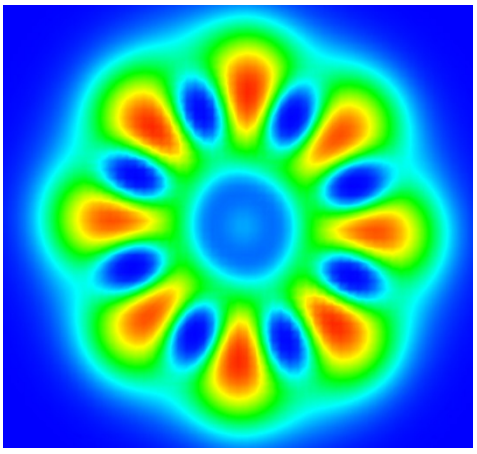
in_Co©B_{16}





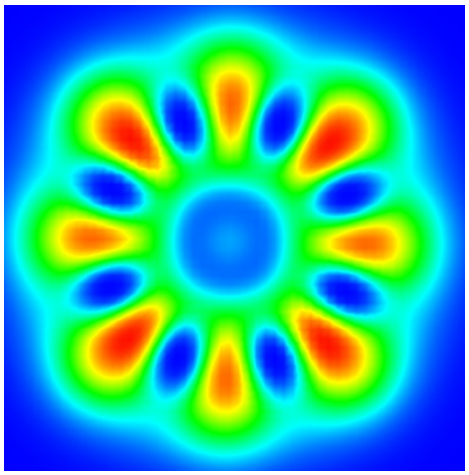
in_Cr©B_{16}



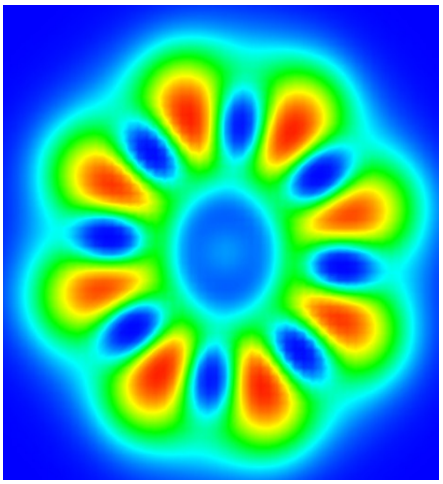


in_Fe©B_{16}

negative



neutral

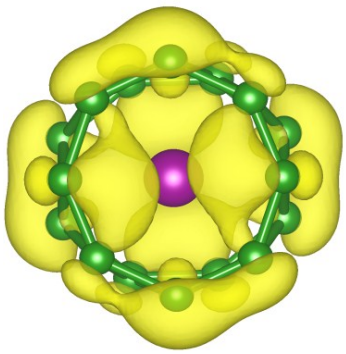


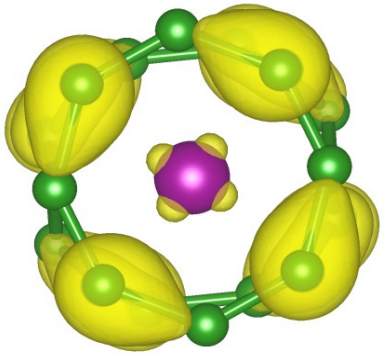
in_Mn©B_{16}

Figure S4: Contour plots of ELF for negative (q=-1) and neutral (q=0) most stable structure of M©B_{16} clusters computed at HSE06 level of theory.

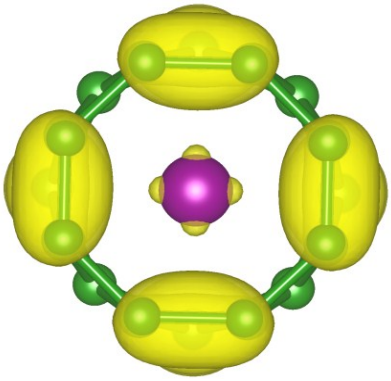
H L

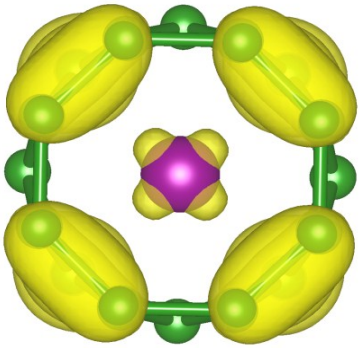
Q=0





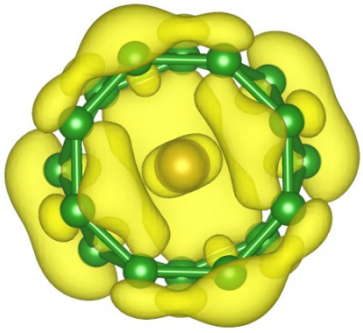
Q=-1

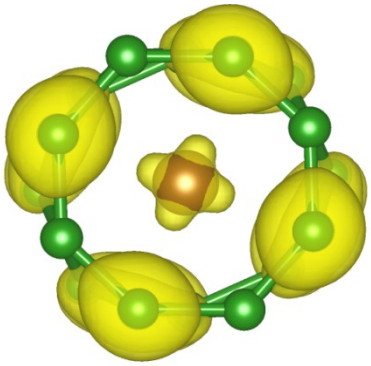




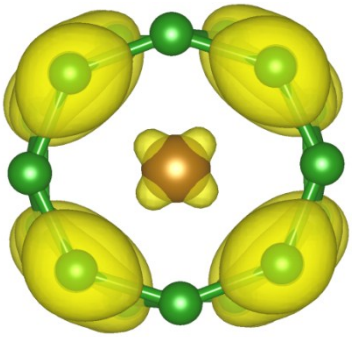
in_Mn©B_{16}

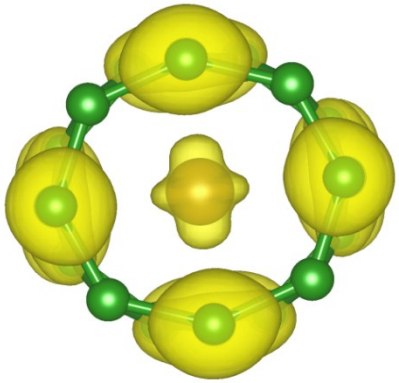
Q=0





Q=-1





in_Fe©B_{16}

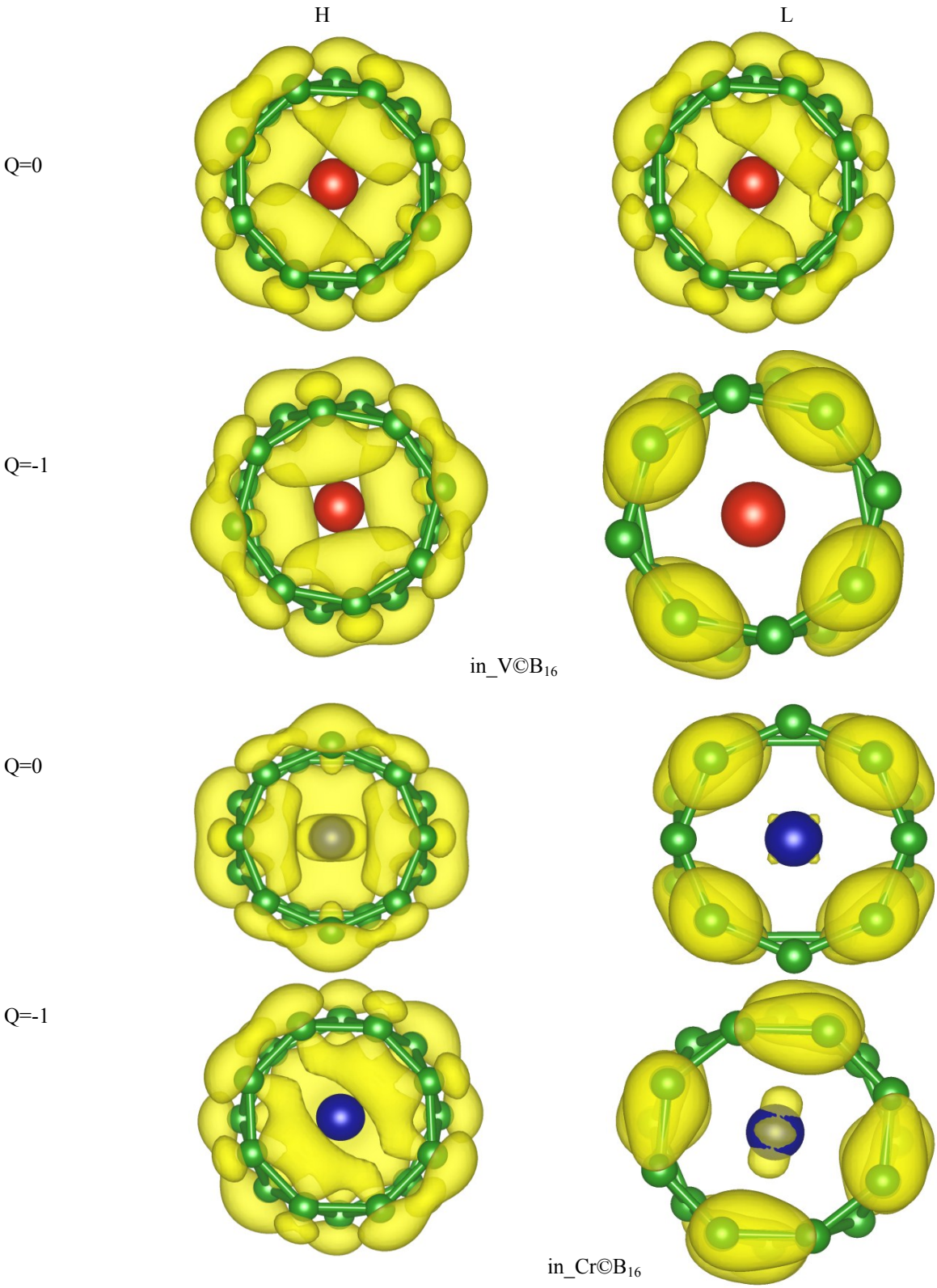


Figure S5: HSE06-DFT calculated contour plots of HOMO and LUMOs orbitals of neutral (Q=0) and negative (Q=-1) most stable structure of Mn©B_{16} and Fe©B_{16} clusters.