

Supporting Information

Structural, optical and hydrogen adsorption properties of B_9 /metal- B_9 clusters: A Density Functional Theoretical Study

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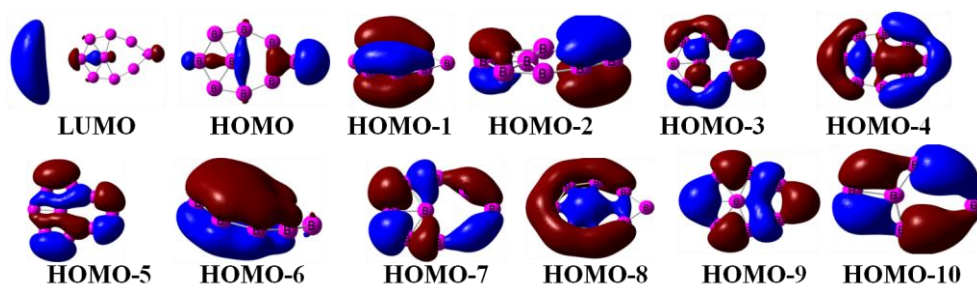


Figure S1 Molecular Orbital representations, involved in delocalization and structural framework for B_9^{3-} conformer-A, are given.

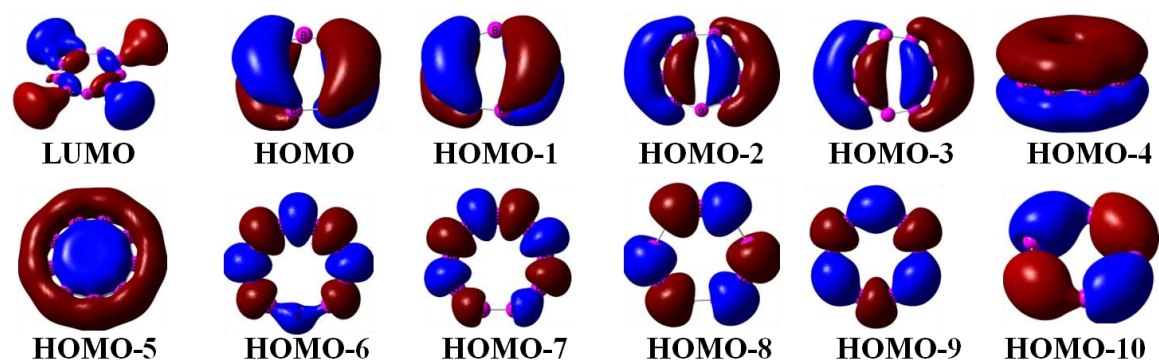


Figure S2 Molecular Orbital representations, involved in delocalization and structural framework for B_9^{3-} conformer-C are given.

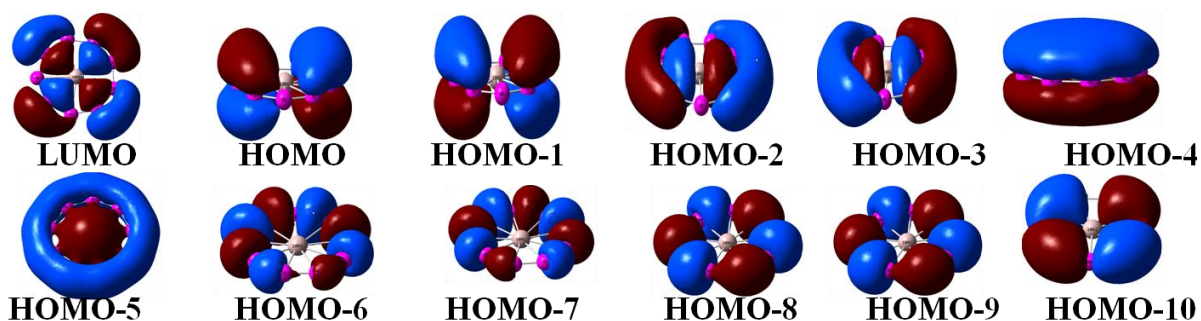


Figure S3 Molecular Orbital representations, involved in delocalization and structural framework for GM@ B_9 are given.