Supporting Information

Structural, optical and hydrogen adsorption properties of B<sub>9</sub>/metal-B<sub>9</sub> clusters: A Density Functional Theoretical Study

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Figure S1 Molecular Orbital representations, involved in delocalization and structural framework for B<sub>9</sub><sup>3−</sup> 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.