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Atomic Clusters: A Unique Building Motif for Future Smart Nanomaterials

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Abstract : The fundamental issue in understanding the origin and growth mechanism of nanomaterials, from a fundamental unit is a big challenging problem to the scientists. Recently, an immense attention is generated to the researchers for prediction of exceptionally stable atomic cluster units as the building units for future smart materials. The present study is a systematic investigation on the stability and electronic properties of a series of bimetallic (semiconductor-alkaline earth) clusters, viz., BxMg3 (x=1-5) is performed, in search for exceptional and/ or unusual stable motifs. A very popular hybrid exchange-correlation functional, B3LYP as proposed by A. D. Becke along with a higher basis set, viz., 6-31+G[d,p] is employed for this purpose under the density functional formalism. The magic stability among the concerned clusters is explained using the jellium model. It is evident from the present study that the magic stability of B4Mg3 cluster arises due to the jellium shell closure.

Keywords : atomic clusters, density functional theory, jellium model, magic clusters, smart nanomaterials
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