POLYHEDRAL HETEROBORANE QUANTUM CHEMISTRY

Josep M. Oliva
Instituto de Química-Física “Rocasolano” (CSIC)
C/Serrano, 119, Madrid 28006, Spain
J.M.Oliva@iqfr.csic.es

Boron chemistry does not have the simplified detailed understanding of classical organic chemistry. However, the peculiar electronic structures admitted for boron species yields a rich variety of different interactions which emerge as a voyage between the worlds of organic, inorganic, and metal chemistry. Here, we report on reaction mechanisms and properties of monomeric, dimeric and other (hetero)borane clusters in their ground and excited electronic states, as a base for predicting the properties of complex polyhedral boron-based molecular architectures, especially based upon the $B_{12}H_{12}^{2-}$ moiety.