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On the role of different types of electron in double ring tubular clusters

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Abstract

Partial electron localization functions $\text{ELF}(\sigma_{\text{loca}})$, $\text{ELF}(\pi)$ and $\text{ELF}(\sigma_{\text{delo}})$ of boron B_n and silicon MSi_{12} double ring (DR) clusters were analyzed. In a DR, separated basins are localized within peripheral bonds (σ), delocalized outside inner bonds (π), or delocalized above and below peripheral bonds (σ). MO spectrum of skeleton D_{6h} Si_{12} DR follows delightfully the hollow cylinder model. A mixture of different sets of MOs makes the D_{6h} Si_{12} structure highly unstable. Upon interacting with $3d$ orbitals of Cr dopant, such a mixed behavior of MO sets is removed and the Cr@Si_{12} DR becomes a global minimum structure.

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