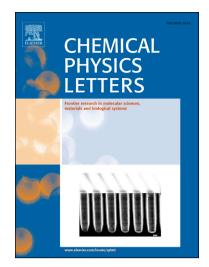
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Research paper

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

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ACCEPTED MANUSCRIPT

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

clusters

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Abstract

Partial electron localization functions $\text{ELF}(\sigma_{0} \text{loca})$, $\text{ELF}(\pi)$ and $\text{ELF}(\sigma_{0} \text{delo})$ of boron B_n and silicon MSi₁₂ 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} Si₁₂ DR follows delightfully the hollow cylinder model. A mixture of different sets of MOs makes the D_{6h} Si₁₂ structure highly unstable. Upon interacting with 3*d* orbitals of Cr dopant, such a mixed behavior of MO sets is removed and the Cr@Si₁₂ DR becomes a global minimum structure.

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