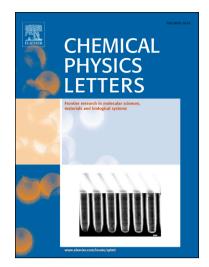
## Accepted Manuscript

#### 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<sub>n</sub> and silicon MSi<sub>12</sub> double ring (DR) clusters were analyzed. In a DR, separated basins are localized within peripheral bonds ( $\sigma$ ), delocalized outside inner bonds ( $\pi$ ), or delocalized above and below peripheral bonds ( $\sigma$ ). MO spectrum of skeleton  $D_{6h}$  Si<sub>12</sub> DR follows delightfully the hollow cylinder model. A mixture of different sets of MOs makes the  $D_{6h}$  Si<sub>12</sub> structure highly unstable. Upon interacting with 3*d* orbitals of Cr dopant, such a mixed behavior of MO sets is removed and the Cr@Si<sub>12</sub> DR becomes a global minimum structure.

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