

Toward understanding the electron density distribution in magnetic clusters : insight from the ELF and AIM analyses of ground-state Fe₄.

Autorzy

Sławomir Berski

G. L. Gutsev

M. D. Mochena

Juan Andrés

Rok wydania

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Streszczenie

Topological analysis of the electron localization function (ELF) in the ground-state Fe₄ cluster reveals different regions of valence electron localization in terms of monosynaptic $V(\text{Fe}_i)$, disynaptic $V(\text{Fe}_i, \text{Fe}_j)$, trisynaptic $V(\text{Fe}_i, \text{Fe}_j, \text{Fe}_k)$, and tetrasynaptic $V(\text{Fe}_1, \text{Fe}_2, \text{Fe}_3, \text{Fe}_4)$ bonding valence attractors and basins. The degree of electron localization is found to be smaller than in a homogeneous electron gas with $\eta(\mathbf{r}) \leq 0.490$. A relative fluctuation of the electron density in the valence basins ranges between 0.83 and 0.96, which indicates a rather substantial delocalization of the electron density. Approximately three valence α -electrons are localized at each iron core $C(\text{Fe}_{i=1,4})$ while two α -electrons, i.e., 0.5 e per one atom, are delocalized over the cluster. The valence electrons show a trend toward localization between iron sites and in the proximity of triangular faces of the cluster with the basin population of one electron. Metallic bonds in Fe₄ may be characterized as partially covalent and highly delocalized both spatially and electronically, which is reflected by a large number of local maxima and relatively large fluctuations, respectively.

Słowa kluczowe

Electron density, Quantum mechanics, Molecular orbitals,
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