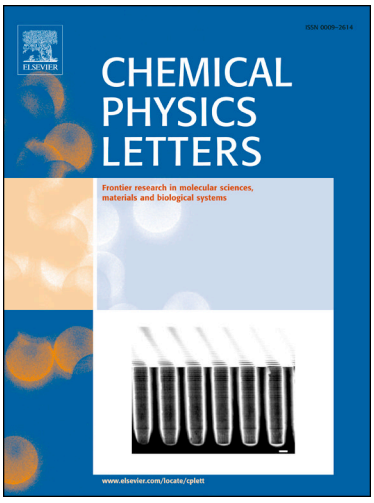

Research paper

Global and local approaches to population analysis: bonding patterns in superheavy element compounds

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Global and local approaches to population analysis: bonding patterns in superheavy element compounds

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Abstract

Relativistic effective atomic configurations of superheavy elements Cn, Nh and Fl and their lighter homologues (Hg, Tl and Pb) in their simple compounds with fluorine and oxygen are determined using the analysis of local properties of molecular Kohn-Sham density matrices in the vicinity of heavy nuclei. The difference in populations of atomic spinors with the same orbital angular momentum and different total angular momenta is demonstrated to be essential for understanding the peculiarities of chemical bonding in superheavy element compounds. The results are fully compatible with those obtained by the relativistic iterative version of conventional projection analysis of global density matrices.

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