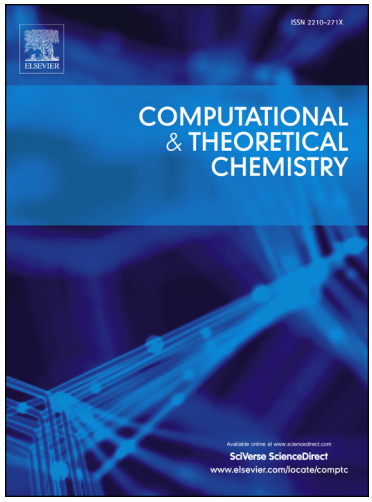

Investigation of structures and energy properties of molybdenum carbide clusters: insight from theory

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Investigation of structures and energy properties of molybdenum carbide clusters: insight from theory

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Density functional theory calculations for $(Mo_2C)_n$ clusters with n=1-10 are presented. For this study the linear combination of Gaussian-type orbitals auxiliary density functional theory (LCGTO-ADFT) approach has been employed. For each cluster size several dozens of isomers, considering different spin multiplicities were studied to determine the lowest energy structures. Initial starting structures for subsequent geometry optimization were taken along Born-Oppenheimer molecular dynamics (BOMD) simulations at different temperatures. This represents the first systematic study on these clusters based on non-symmetry adapted first-principle calculations. Ground state structures, relative stability energy, vibrational frequencies, dissociation energies, ionization potentials, electron affinities and spin density plots are reported. The analysis of the evolution of the ground state structures with increasing the cluster size demonstrates that these systems are characterized by peculiar structure motives and that interesting structure transitions occur at certain system sizes. The comparison of the obtained results with the experimental data from the bulk reveals that packing effects in these clusters can be observed already at very small system size.

Keywords: Molybdenum Carbide Clusters, ADFT, Structures, Born-Oppenheimer molecular dynamics (BOMD) simulations.

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