

Accepted Manuscript

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

Domingo Cruz-Olvera, Patrizia Calaminici

PII: S2210-271X(15)00500-9
DOI: <http://dx.doi.org/10.1016/j.comptc.2015.12.019>
Reference: COMPTC 2023

To appear in: *Computational & Theoretical Chemistry*

Received Date: 10 December 2015
Revised Date: 18 December 2015
Accepted Date: 18 December 2015

Please cite this article as: D. Cruz-Olvera, P. Calaminici, Investigation of structures and energy properties of molybdenum carbide clusters: insight from theory, *Computational & Theoretical Chemistry* (2015), doi: <http://dx.doi.org/10.1016/j.comptc.2015.12.019>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



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

Domingo Cruz-Olvera, Patrizia Calaminici*

Departamento de Química, CINVESTAV

Av. Instituto Politécnico Nacional 2508

AP 14-740, México D.F. 07000 México

Density functional theory calculations for $(\text{Mo}_2\text{C})_n$ 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.

* **Corresponding author:** pcalamin@cinvestav.mx

Download English Version:

<https://daneshyari.com/en/article/5392930>

Download Persian Version:

<https://daneshyari.com/article/5392930>

[Daneshyari.com](https://daneshyari.com)