

A density-functional study of the electronic properties of small Mo clusters

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Abstract

We report the results of *ab initio* calculations of the structures, binding energies and magnetic moments of the clusters Mo_N ($N=2-13$) that were performed using the fully unconstrained version of the density-functional method SIESTA with the generalised gradient approximation to exchange and correlation. We obtain collinear magnetic structures in all cases, even when the self-consistent calculations were started from non-collinear inputs. Our results for the Mo_N clusters show that both linear, planar and three-dimensional clusters have a strong tendency to form dimers. In general, even-numbered clusters are more stable than their neighboring odd-numbered clusters because they can accommodate an integer number of tightly bounded dimers. As a consequence, the binding energies of the Mo_N clusters, in their lowest-energy states, exhibit an odd-even effect in all dimensionalities. Odd-even effects are less noticeable in the magnetic moments than in the binding energies. When comparing our results for Mo clusters with those obtained recently by other authors, we observe similarities in some cases, but striking differences in others. In particular, the odd-even effect in three-dimensional Mo clusters was not observed before, and our results for some clusters (e.g., for planar Mo_3 and Mo_7 and for three-dimensional Mo_7 and Mo_{13}) differ from those reported by other authors.

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