

# *Ab initio* molecular dynamics simulations of 13-atom metal clusters

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## abstract

Atomic geometries, electronic structures, and magnetic moments of several metal clusters with 13 atoms are studied by *ab initio* density-functional calculations. The ground state structures of 13-atom metal clusters were previously assumed to be icosahedron, cuboctahedron, or decahedron. However, in this study, using *ab initio* molecular dynamics simulations, we find another low-lying energy state with a buckled bi-planar structure that has  $C_{2v}$  symmetry. The spin magnetic moments for the buckled bi-planar structure are usually lower than for the icosahedral structure, which are more consistent with existing experimentally measured values. This novel buckled bi-planar structure of 13-atom cluster should be a common low-lying energy state for the late transition metals (with d electrons more than half filled).