Comparative study of metal clusters by Quantum Monte Carlo method

Yuning Wu and Hai-Ping Cheng
Department of Physics, University of Florida, USA
Paul Kent
Oak Ridge National Lab, USA

Lithium and sodium clusters have been studied by fixed-node diffusion quantum Monte Carlo method. This stochastic wave-function-based approach can provide more accurate results and serve as benchmarks against which other techniques may be compared. We studied the binding energies and investigate different geometries to decide the ground state. Our results are compared with those derived from other method such as DFT and CI methods. Our objective is to validate current quantum Monte Carlo methods for small metal clusters that undergo size dependent geometrical transitions.

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