

Abstract Submitted
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Studies of materials from simple metal atoms by quantum Monte Carlo methods KEVIN RASCH, LUBOS MITAS, North Carolina State University — We carry out quantum Monte Carlo (QMC) calculations of systems from simple metal elements such as Li and Na with the goal of studying the cohesive/binding energies, structural characteristics as well as the accuracy of QMC methods for these elements. For Na we use test small-core pseudo potentials vs large-core pseudopotentials with the core polarization and relaxation correction potentials. We test orbital sets from several DFT functionals in order to assess the accuracy of the corresponding wave functions and fixed-node biases. It turns out that the valence correlations energies are very accurate, typically, 97% or higher in most of the tested systems. This provides a validation framework for further QMC studies of these systems in non-equilibrium conformations and at high pressures.

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