The Equations of State of a Wide Range of Solids Using the AFQMC and FCIQMC Methods

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We compute the equations of state of a variety of solids using the Auxiliary Field (AFQMC) [1] and Full Configuration Interaction (FCIQMC)[2] Quantum Monte Carlo methods. These recently developed techniques have previously been shown to be promising routes for obtaining the electronic structure of strongly correlated atoms and molecules, but have not been widely applied to solids. We explore the capabilities of the methods on a broad class of solids with different chemical bonding. We find that the equilibrium lattice constants they predict are in good agreement with experimental results.

[1] S. Zhang, "Auxiliary-Field Quantum Monte Carlo for Correlated Electron Systems, Emergent Phenomena in Correlated Matter, Modeling and Simulation Vol. 3 (2013), Edtied by E. Pavarini, E. Koch, and U. Schollwock.
[2]G.H. Booth, A. Gruneis, A. Alavi, Nature 493, 365–370 Jan 2013.