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Exploring AFQMC Calculations in Solids and Molecules EDGAR JOSUE LANDINEZ BORDA, MIGUEL MORALES SILVA, Lawrence Livermore National Lab, BRENDA RUBENSTEIN COLLABORATION[1], JOHN GOMEZ COLLABORATION[2] — The Auxiliary Field Quantum Monte Carlo (AFQMC) [1] method has been outlined as a promising path to compute the electronic structure of strong correlated molecules and solids [2],[3]. We explore its capabilities in a broad range of solids and molecules with different types of chemical structure and bonding. In addition, we study the use of single and non-orthogonal multi-determinant wave functions [4] in the calculation of of the equation of state and atomization energies of the systems studied. Overall, we finding good agreement with experimental results.\[1]Shiwei Zhang, Henry Krakauer, Phys. Rev. Lett. 90. 136401 (2003). \f0 [2] 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.\f0 [3] Fengjie Ma, Wirawan Purwanto, Shiwei Zhang, and Henry Krakauer Phys. Rev. Lett. 114, 226401 (2015)\f0 [4]Symmetry-projected wavefunctions in Quantum Monte Carlo calculations, H. Shi, C. A. Jiménez-Hoyos, R. R. Rodríguez-Guzmán, G. E. Scuseria, and S. Zhang,Phys. Rev.B 89, 125129 (2014).

[1]Brown University
[2]Rice University

Edgar Josue Landinez Borda
Lawrence Livermore National Lab

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