Forces, stress, and geometry optimization with auxiliary-field quantum Monte Carlo

Determining the accurate structure of a material is a critical step in understanding its physics. Predictive computations in correlated materials remain a major challenge. We have successfully formulated and implemented a direct, ab initio computation of forces and stresses [1] with auxiliary-field quantum Monte Carlo (AFQMC) using plane wave basis and multiple projector pseudopotentials. Our method potentially allows determination of the potential energy surface at a much higher efficiency than an approach based on total energies alone. In addition, we propose a fast and robust structural optimization algorithm [2] for optimizations when the forces or gradients are statistically noisy. Applying this algorithm in combination with forces and stresses computed by AFQMC, we demonstrate efficient, accurate, and full degrees-of-freedom optimizations in solids. Direct computations of charge densities [3], phonon spectra, and Berry phases in solids with AFQMC will also be discussed.

[1] S. Chen and S. Zhang, arXiv:2302.07460, to appear on Phys. Rev. B
[2] S. Chen and S. Zhang, Nat. Comput. Sci. 2, 736 (2022)
[3] S. Chen, M. Motta, F. Ma, and S. Zhang, Phys. Rev. B 103, 075138 (2021)