Auxiliary-Field Quantum Monte Carlo Studies of Pressure-Induced Phase Transitions in Silicon and MnO\textsuperscript{1} WIRAWAN PURWANTO, HENRY KRAKAUER, ERIC WALTER, SHIWEI ZHANG, College of William and Mary — Accurate theoretical predictions across structural phase transitions are challenging, as they typically involve different electronic structures on the two sides of the transition. We use the phaseless auxiliary-field quantum Monte Carlo (AFQMC) method—which yields accurate many-body wave functions by means of importance sampled random walks in the space of Slater determinants—to calculate the equation of state near two phase transitions: in Si, from the diamond to metallic \(\beta\)-tin transition at \(\sim 11\) GPa; and in MnO, the volume and magnetic moment collapse at \(\sim 100\) GPa. The Si phase transition serves as a test case to study the accuracy of the AFQMC method; the calculated transition pressure is in good agreement with the experiment. Applications to the MnO phase transition will then be presented.

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