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Quantum Monte Carlo calculations of structural and electronic properties in the correlated oxide NiO[1] CHANDRIMA MITRA, JARON KROGEL, JUAN A. SANTANA PALACIO, FERNANDO A. REBOREDO, Oak Ridge National Laboratory — Transition metal oxides pose difficulties for condensed matter theories due to the presence of strong electronic correlations. The complex interplay among correlation and exchange in d subshells, crystal field effects, p-d hybridization and charge transfer gives rise to a rich variety of structural and electronic phases. NiO is one such challenging d system, where conventional band theory fails. Compared to the experimental value, the cohesive energy of bulk NiO computed within DFT-LDA differs by almost a factor of 18 %. Band gap computed within standard local or semi-local functionals are off by a factor of 80 %. A quasi-particle correction like the G^0W^0 approach cannot correct the band gap and is still by far too low. In this work we adopt the Diffusion Quantum Monte (DMC) approach to study the structural and electronic properties of NiO. Trial wave-functions were self consistently generated in a Slater-Jastrow form. To test pseudopotentials used, DMC calculations were done on atomic Ni and O and their computed ionization potentials showed excellent agreement with experiments (within 0.04%). The equilibrium bond length and binding energy of the NiO dimer were also computed that were 0.001% and 0.03%, respectively, from experimental values. DMC calculations of equation of state and band gap of bulk NiO will be presented.

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