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Study of TiO and MnO using auxiliary field quantum Monte Carlo[1] WISSAM AL-SAIDI, HENRY KRAKAUER, SHIWEI ZHANG, College of William and Mary — We study the transition metal oxide molecules TiO and MnO using the recently developed auxiliary field quantum Monte Carlo approach [1]. This method maps the interacting many-body problem into a linear combination of non-interacting problems using a complex Hubbard-Stratonovich transformation, and controls the phase/sign problem using a trial wave function. It employs a random walk approach in Slater determinant space to project the ground state of the system, and uses much of the same machinery as density functional theory such as single particle basis and non-local pseudopotentials. In our calculations, we used a single Slater determinant trial wave function obtained from a density functional calculation, with no further optimization. The calculated dissociation energies are in good agreement with experiments. These together with previous results show the robustness of the method for studying sp- as well as d-bonded atoms, and molecules. Calculations of other observables and correlation functions will also be discussed. [1] S. Zhang and H. Krakauer, Phys. Rev. Lett. 90, 126401 (2003).

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