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Quantum Monte-Carlo Study of Mn and Mn-oxide clusters. HIORI KINO, LUCAS K. WAGNER, LUBOS MITAS, Department of Physics, North Carolina State Univ., NATIONAL INSTITUTE FOR MATERIALS SCIENCE, JAPAN COLLABORATION — Many molecules and clusters of Mn and Mn-oxide have not only interesting physical properties but also can be found in enzymes as important components in biochemical reactions. The electronic structure calculations of these systems are difficult and, for example, choice of exchange-correlation functionals in Density Functional Theory can significantly influence both ground state geometries and spin-state predictions. Therefore, highly accurate calculation is very desirable for these systems. Experimentally, it is established that the Mn dimer is a van der Waals system with weak binding, however, the spin multiplicity has not been settled unambiguously with possibilities covering a range from singlet, triplet, etc, up to 2S+1=11. On the other hand, Mn_nO_n molecules are quite well understood as being a high-spin system, but their geometries depend on the exchange-correlation functionals. We will present our recent results from the fixed-node quantum Monte Carlo calculations of these systems. We will also report on recent progress in modeling the [4Mn-4O-Ca] cluster structural prototypes for the oxygen evolving center in green plants Photosystem II.

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