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Lattice Regularized Diffusion Monte Carlo Simulations of iron dimer MICHELE CASULA, Department of Physics, University of Illinois at Urbana-Champaign, 1110 W. Green Street, Urbana, Illinois 61801, USA, LEONARDO GUIDONI, Universita' degli Studi di Roma "La Sapienza", Physics Department,, SANDRO SORELLA, International School for Advanced Studies (SISSA), Via Beirut 2-4, 34014 Trieste, Italy — Transition metal compounds play a crucial role in various fields, ranging from biomolecular reactions to magnetic solid state properties. On the other hand, the strong dynamic correlation present in the unfilled d-shell makes the predictions of the density functional theory unreliable and requires the use of post-Hartree-Fock methods, limited however to small systems. The Lattice Regularized Diffusion Monte Carlo (LRDMC) method, recently introduced [M. Casula, C. Filippi, and S. Sorella, Phys. Rev. Lett. 95, 100201 (2005)], seems to be an effective alternative, since it can provide accurate results with a favorable size scaling. One of the main advantages of this framework is the possibility to include non-local potentials in a consistent variational scheme, substantially improving both the accuracy and the computational stability upon previous non-variational diffusion Monte Carlo approaches. Here, we apply the LRDMC framework to the iron dimer, by using a fully optimized Jastrow geminal wave function as guiding state. Despite its simplicity, its neutral and anionic ground states are controversial, and we try to clarify their symmetry by comparing our LRDMC results with experimental spectroscopic data.

Michele Casula
Department of Physics, University of Illinois at Urbana-Champaign,
1110 W. Green Street, Urbana, Illinois 61801, USA

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