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Low energy model estimation from detailed quantum Monte Carlo calculations for transition metal systems[1] LUCAS WAGNER, University of Illinois at Urbana-Champaign — Systems of strongly correlated electrons have incredible potential for new devices and new quantum states. However, it is very challenging to a priori predict the quantum state of a system of correlated electrons. Detailed calculations using quantum Monte Carlo methods on the first principles Hamiltonian have in recent years shown to be quite reliable for some example transition metal oxide systems, such as FeO, ZnO, among others. These calculations, although they are accurate, have not provided much information in terms of the correct approximate low-energy model that should describe the systems in question. In this talk, I'll summarize the results of matching the two-body correlations from first principles quantum Monte Carlo on transition metal systems to models and discuss the implications for the commonly used models.

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Lucas Wagner
University of Illinois at Urbana-Champaign

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