

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

An ab initio approach to the origin of superexchange¹ ALEXANDER MUNOZ, LUCAS K. WAGNER, University of Illinois, Urbana-Champaign — The superexchange mechanism is the traditional explanation for antiferromagnetic couplings between magnetic ions. In this theory, the energy savings within the context of a hopping model is derived from kinetic energy terms. Our study focuses on determining, from ab initio calculations, whether the origin of interactions in magnetic systems is explainable through the conventional arguments. Using quantum Monte Carlo, we investigate the model system $(\text{Mn-O-Mn})^{+2}$ where we will report on progress establishing the ab initio explanation for superexchange. We will focus on elucidating the ab initio calculated correlators and the effective model energy savings that result in an antiferromagnetic interaction in this system.

¹Funding for this research was provided by the National Center for Supercomputing Applications and the College of Engineering at the University of Illinois, Urbana-Champaign

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Date submitted: 11 Nov 2016

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