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Computation of ab initio energy savings due to magnetic interactions[1] ALEXANDER MUNOZ, LUCAS WAGNER, Univ of Illinois - Urbana — The double-exchange mechanism [1] is the traditional explanation for antiferromagnetic coupling between magnetic ions. In this theory, the energy savings within the context of a hopping model is derived from kinetic energy terms. However, the connection to ab initio energy savings to our knowledge has not been studied using an explicitly correlated theory that can obtain quantitative accuracy. Our study focuses on determining, from ab initio calculations, whether the origin of interactions in magnetic systems is explainable through conventional arguments. To this end, we investigate the contributions (kinetic, ionic, electron-electron) to the total energy of the $(Mn\text{-}O\text{-}Mn)^{+2}$system using quantum Monte Carlo techniques. We will report on progress in elucidating the connection between the ab initio energy savings and the effective model energy savings that result in an antiferromagnetic interaction in this system. [1] Zener. Phys. Rev. , 403 (1951)

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Alexander Munoz
Univ of Illinois - Urbana

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