

Abstract Submitted
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Spin and Orbital fluctuations in antiferromagnetic RbO₂ ERIK YLVISAKER, RAJIV SINGH, WARREN PICKETT, UC Davis — We examine magnon and orbiton behavior in the Mott insulating RbO₂, where the magnetic moment is confined to localized O₂ anti-bonding molecular π^* orbitals, and the orbital ordering is frustrated. We derive an effective Kugel-Khomskii Hamiltonian from a two band Hubbard model with hopping parameters taken from *ab initio* density functional calculations. The ground state orbital order is frustrated, and due to the rather different interband and intraband hoppings this leads to a magnon excitation spectrum which is strongly dependent on the orbital ground state. This strong coupling between the magnon spectrum and the orbital ground state, along with the near degeneracy of the orbital ordering leads to a quenching of the spin order, resulting in a Néel temperature significantly lower than mean field theory predicts.

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