Abstract Submitted
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**Hybridization wave as the cause of the metal-insulator transition in rare earth nickelates**[1] HYOWON PARK, Department of Physics, Columbia University, CHRIS A. MARIANETTI, Department of Applied Physics, Columbia University, ANDREW J. MILLIS, Department of Physics, Columbia University — The metal-insulator transition driven by varying rare earth ($Re$) ion in $ReNiO_3$ has been a longstanding challenge to materials theory. Experimental evidence suggesting charge order is seemingly incompatible with the strong Mott-Hubbard correlations characteristic of transition metals. We present density functional, Hartree-Fock and Dynamical Mean field calculations showing that the origin of the insulating phase is a hybridization wave, in which a two sublattice ordering of the oxygen breathing mode produces two $Ni$ sites with almost identical $Ni$ $d$-charge densities but very different magnetic moments and other properties. The high temperature crystal structure associated with smaller $Re$ ions such as $Lu$ is shown to be more susceptible to the distortion than the high temperature structure associated with larger $Re$ ions such as $La$.

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