A realistic approach to effective Hamiltonians for strongly correlated electron materials: Study of orbital ordering in LaMnO$_3$\textsuperscript{1} WEI-GUO YIN, DMITRI VOLJA, WEI KU, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973 — We present a general scheme to the realistic derivation of many-body effective Hamiltonians, $H^{\text{eff}}$, for strongly correlated electron systems: Based on a novel Wannier state analysis of the LDA+$U$ electronic structure, relevant mechanisms can be clearly singled out and their strengths can be accurately determined by mapping $H^{\text{eff}}$ to the low-energy LDA+$U$ Hamiltonian within self-consistent Hartree-Fock mean-field theory \cite{1}. Applying this scheme to LaMnO$_3$, the parent compound of colossal magnetoresistance manganites, we have quantified the relative importance of the effective electron-electron interaction ($\sim 1.7$ eV) and the Jahn-Teller splitting ($\sim 0.9$ eV) in ordering orbitals in LaMnO$_3$. We find that beyond the conventional Jahn-Teller picture, the electron-lattice (electron-electron) interaction alone is insufficient (sufficient) to stabilize the orbital ordering. Furthermore, our analysis indicates certain competition between different mechanisms, allowing direct experimental determination of their relative strengths. \cite{1} W.-G. Yin, D. Volja, and W. Ku, cond-mat/0509075.

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