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Calculation of model Hamiltonian parameters for $LaMnO_3$ using maximally localized Wannier functions ROMAN KOVACIK, CLAUDE EDERER, School of Physics, Trinity College Dublin, Ireland — The theoretical description of transition metal oxides is often based on effective tight-binding (TB) models. A systematic way to obtain realistic TB models is the construction of maximally localized Wannier functions (MLWFs) [1]. The corresponding TB representation is given by the real space Hamiltonian matrix elements in the MLWF basis. Here, we construct MLWFs for the Mn e_g bands in $LaMnO_3$, and we monitor changes in the MLWF matrix elements induced by different magnetic configurations and structural distortions. From this we obtain values for the local Jahn-Teller and Hund's rule coupling strength, the hopping amplitudes between all nearest and further neighbors, and the corresponding reduction due to the $GdFeO_3$-type distortion. By comparing our results with commonly used model Hamiltonians for manganites, where electrons can hop between two "e_g-like" orbitals located on each Mn site, we find that the most crucial limitation of such models stems from neglecting changes in the underlying Mn(d)-O(p) hybridization. [1] N. Marzari and D. Vanderbilt, Phys. Rev. B 56, 12847 (1997).

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