Calculation of maximally localized Wannier functions and hopping parameters for $LaMnO_3$

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Strong electronic correlations lead to rich phase diagrams of electronic and magnetic states for many transition-metal oxides. $LaMnO_3$ is one of the prototype materials to study the resulting phenomena such as for example colossal magnetoresistance. The widely used local density approximation (LDA) to density functional theory (DFT) fails to correctly describe correlated-electron systems. Therefore, a lot of effort is put into the development of novel methods such as LDA+DMFT, which combines DFT with many-body techniques (dynamical mean-field theory). The representation of electrons using Wannier functions is well suited to link these two approaches.

$LaMnO_3$ crystallizes in an orthorhombically distorted perovskite structure with Jahn-Teller (JT) and $GdFeO_3$-type (GFO) distortions of MnO_6 octahedra. The magnetic moments ordering of the Mn cations is antiferromagnetic (A-type). Using the DFT-based PWscf program (www.pwscf.org) we calculate electronic structure of different $LaMnO_3$ model systems (see below), which is further processed using the wannier90 program (www.wannier.org) to obtain maximally localized Wannier functions (MLWF).[1]

To understand the influence of the structural distortions on electronic properties, we set up several model atomic structures: the simple cubic, purely JT- and purely GFO-distorted, and the full experimental structure. For each of them we investigate two cases: effective Mn(d) 2-e_g-band model and full Mn(d)+O(p)-band model. We briefly discuss convergence of data as a function of k-point mesh and optimization techniques. The construction of MLWF using the disentanglement procedure[1] is found to perform very well even for strongly entangled bands. Furthermore, we analyze hopping parameters and compare them with the widely used 2-band tight-binding model (see e.g. Ref. 2).

[1] I. Souza, N. Marzari, and D. Vanderbilt, Phys. Rev. B **65**, 035109 (2001).

[2] C. Ederer, C. Lin, and A.J. Millis, Phys. Rev. B **76**, 155105 (2007).