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Maximally localized Wannier functions in $LaMnO_3$ within PBE+U, hybrid functionals, and GW: an efficient route to construct ab-initio tight-binding parameters for e_g perovskites ROMAN KOVACIK, School of Physics, Trinity College Dublin, Dublin 2, Ireland, CESARE FRANCHINI, MARTIJN MARSMAN, Faculty of Physics, University of Vienna and Center for Computational Materials Science, A-1090 Wien, Austria, CLAUDE EDERER, School of Physics, Trinity College Dublin, Dublin 2, Ireland — Using the newly developed VASP2WANNIER90 interface we have constructed maximally localized Wannier functions [1] (MLWFs) for the e_g states of the prototypical Jahn-Teller magnetic perovskite $LaMnO_3$ at different levels of approximation for the exchange-correlation kernel. These include conventional density functional theory (DFT) with and without additional on-site Hubbard U term, hybrid-DFT, and single shot GW. By suitably mapping the MLWFs onto an effective e_g tight-binding (TB) Hamiltonian [2,3] we have computed a complete set of TB parameters providing the band dispersion in excellent agreement with the underlying *ab initio* and MLWF bands. The method-dependent changes of the TB parameters and their interplay with the electron-electron interaction term are discussed and interpreted, outlining a guidance for more elaborate treatments of correlation effects in effective Hamiltonian-based approaches.
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Roman Kovacik
School of Physics, Trinity College Dublin, Dublin 2, Ireland

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