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Hybrid functionals for simulating complex oxides

CESARE FRANCHINI, University of Vienna

Hybrid functionals are a class of exchange-correlation (XC) functionals in density functional theory (DFT) that are constructed by a suitable mixing of local/semi-local XC functionals (LDA/GGA) with a certain portion of the exact Hartree-Fock exchange. After being used for years in the chemistry community for studying molecular properties, hybrid functionals are being increasingly widely used for solid state problems, for which standard LDA/GGA approximations provide a defective description. In particular, hybrid functionals appear to account well for the complicated coupling between lattice, charge and spin degrees of freedom in transition metal oxides, a class of materials that has recently attracted a lot of interest due to its technological relevance (all-oxides electronics), the large spectrum of functionalities, and the many challenging issues related to strong electronic correlation [1,2]. The purpose of this talk is to present the essential ideas and physical picture of hybrid functionals and to present a map of recent applications to complex oxides aiming to cover an ample spectra of cases (sp, $3d$, $4d$ and $5d$ compounds) and to discuss an extended array of physical phenomena including: metal-to-insulator transitions, electron localization, bandgap prediction, polarons, multiferroism, and spin-orbit coupling. [1] C. Franchini, J. Phys. Condens. Matter 26, 253202 (2014). [2] J. G. He and C. Franchini, Phys. Rev. B 86, 235117 (2012).