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【505】Transition-metal compounds from extended Hubbard functionals

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An accurate modeling of transition-metal compounds is central to many scientific problems and technological applications including battery materials, photovoltaics, multiferroics, superconductors.
Unfortunately, approximate DFT functionals do not capture electronic localization in low-dispersion states (e.g., d or f) and misrepresent important properties of these systems.
This work shows how extended Hubbard corrections to current functionals, including on-site and inter-site interactions, improve dramatically the description of many physical properties, capturing localization even in presence of hybridization. Materials for Li-ion batteries will be used to demonstrate how interaction parameters consistent with the electronic and crystal structures greatly improve the prediction of thermodynamic quantities and average voltages. A new algorithm to evaluate them from density-functional perturbation theory is shown to guarantee efficiency and accuracy.

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