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【625】Hubbard interactions from density-functional perturbation theory

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DFT+U is a simple and powerful tool to model systems containing partially-filled manifolds of localized states. Conceptual and practical methods to determine U ab initio have been introduced long ago, based either on the constrained random-phase approximation or on linear-response theory. However, these approaches are often overlooked due to their cost or complexity. Here, we introduce a computationally efficient approach to determine U, hitherto obtained from the difference between bare and self-consistent inverse electronic susceptibilities evaluated from supercell calculations. By recasting these calculations in the language of density-functional perturbation theory we remove the need of supercells, and allow for a fully automated determination of susceptibilities and Hubbard parameters.

Primary authors: TIMROV, Iurii (Ecole Polytechnique Federale de Lausanne); Dr COCOCCIONI, Matteo (EPFL); Prof. MARZARI, Nicola (EPFL)

Presenter: TIMROV, Iurii (Ecole Polytechnique Federale de Lausanne)

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