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【506】Hubbard interactions from density-functional perturbation theory

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DFT+U+V is a simple and powerful tool to model systems containing partially-filled manifolds of localized states. However, the Hubbard parameters are often treated semi-empirically, which is a somewhat unsatisfactory approach. Conceptual and practical methods to determine e.g. the Hubbard U parameter from first principles have nevertheless been introduced long ago, based either on the constrained random-phase approximation or on linear-response theory. Nonetheless, these approaches are often overlooked due to their cost or complexity. Here, we introduce a computationally inexpensive and straightforward approach to determine on-site U and inter-site V based on density-functional perturbation theory. Such developments open the way for deployment in high-throughput studies, while providing the community with a simple tool to calculate consistent values of U and V.

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