First-principles calculation of Hubbard U within linear response theory in the basis of Wannier functions

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DFT+U is one of the most widely used methods for correcting the self-interaction error of approximate density functionals in systems with localized d or f electrons. However, its predictions depend strongly on the choice of the Hubbard projectors that define the localized manifold. Standard implementations rely on atomic-like projectors, which are not necessarily representative of the states that actually drive the physics of the material. In this talk, I will discuss an alternative approach based on frontier Wannier functions (molecular orbitals), which are constructed from the states near the Fermi level and therefore adapt to the chemical environment of the system. I will compare them with conventional (atomic-like) Hubbard projectors, analyzing the differences in the Hubbard U computed from first principles via linear-response theory and in the resulting ground state, both through a formal derivation and through numerical simulations. I will also present a new implementation in the HP [1] code of Quantum ESPRESSO that enables the first-principles calculation of Hubbard U using Wannier-function projectors, making this approach directly available for routine use. This comparison shows that the choice of projector is not a technical detail but a central ingredient of a predictive DFT+U description, which is as important as the choice of the Hubbard U.

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