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A consistent, linear-response approach to LDA+U

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Hubbard U-correction to LDA or GGA has proven very effective in describing several strongly-correlated systems for which these approximations to DFT otherwise fail.

Constrained DFT or semiempirical approaches have been often used to compute the Hubbard U. I introduce here an alternative scheme to evaluate the effective electronic interaction in a fully consistent way.

This approach is based on the linear response of the system under consideration to a potential shift acting on the localized orbitals of the correlated sites. Using the occupations of these orbitals as the relevant electronic degrees of freedom we compute the on-site electronic coupling as the difference between the inverse of the bare and of the fully-interacting response matrices. The U computed in this way thus corresponds to the effective, atomically-averaged kernel of the Hartree-exchange-correlation interaction, in agreement with the second quantization expression of the "+U" energy functional. In this way the strength of the "+U" correction is evaluated from the same DFT scheme we aim to correct so that LDA+U becomes a consistent non-parametric method, with no need for semiempirical evaluations of the effective coupling.

With this approach we successfully studied the structural, electronic, chemical and electrochemical properties of several transition-metal compounds. Examples will include minerals in the Earth's interior¹, cathode materials for next-generation lithium batteries² and metal-organic complexes³.

- 1) M. Cococcioni and S. de Gironcoli, PRB (2005).
- 2) F. Zhou, M. Cococcioni, A. C. Marianetti, D. Morgan and G. Ceder, PRB (2004).
- 3) H. J. Kulik, M. Cococcioni, D. Scherlis and N. Marzari, submitted to PRL.