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Extended LDA+U+V approach for covalently bonded systems

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A novel DFT+U energy functional (named DFT+U+V) is introduced based on a corrective Hubbard Hamiltonian that includes both on-site (U) and inter-site (V) electron-electron interactions. The competition between these couplings allows for more general localization regimes (e.g., on hybrid, molecular states). Systems as diverse as Mott insulators and covalent semiconductors can be described within the same theoretical framework. Also, phenomena like electron-transfer reactions or formation and breaking of bonds, whose modeling within "standard" (e.g., LDA or GGA) approximations to DFT or with the "on-site" DFT+U approach is problematic, will be addressed with higher precision. Accurate energetics is guaranteed by the consistent evaluation of V that can be obtained, at no additional cost, from the same linear-response approach used to calculate U [1]. The flexibility and reliability of the novel functional are demonstrated by its application to covalent (Si) and ionic (GaAs) semiconductors and to charge-transfer insulators (NiO). [1] M. Cococcioni and S. de Gironcoli, Phys. Rev. B 71, 035105 (2005).

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