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Extended LDA+U+V approach for covalent systems MATTEO COCOCCIONI, Department of Chemical Engineering and Materials Science, University of Minnesota , VIVALDO LEIRIA CAMPO, Departamento de Fisica, Universidade Federal de Sao Carlos, Sao Carlos, Brazil — 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 interactions avoids the over-stabilization of occupied atomic orbitals, usually observed within the "on-site-only" DFT+U approach, and allows to describe systems in which hybridization plays an important role (as, e.g. semiconductors doped with magnetic impurities, or high T$_c$ superconductors) and whose behavior is intermediate between that of Mott and band insulators. In addition, the inter-site interaction parameter V can be straightforwardly 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 prototypical 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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