

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Generalized LDA+U+V functional in DFT calculations for covalent systems VIVALDO CAMPO, MATTEO COCOCCIONI, Chemical Engineering and Materials Science Department, University of Minnesota, Minneapolis, MN 55455, USA — In this work, we introduce a generalized LDA+U+V functional that consists in both on-site (U) and inter-site (V) interactions. While V can be straightforwardly obtained from the same linear-response approach used to calculate U [1], its inclusion in the “+U” energy functional can improve the treatment of systems where electrons tend to localize on molecular states (bonds) rather than on atomic orbitals, and will extend the applicability of this approach to a much broader class of systems. Because of a better treatment of hybridization, this extension also helps avoiding well-known drawbacks of “standard” (atomic) LDA+U such as the exaggerated down-shift of the energy of localized filled orbitals. It thus results in an improved energetic description, which is crucial for studying structural relaxations, chemical reactions and phase transitions. Paradigmatic examples of application of this generalized approach will include diatomic molecules, TM oxides and group-IV solids. ¹ M. Cococcioni and S. de Gironcoli, Phys. Rev. B **71**, 035105 (2005).

Vivaldo Campo
Chemical Engineering and Materials Science Department,
University of Minnesota, Minneapolis, MN 55455, USA

Date submitted: 13 Dec 2007

Electronic form version 1.4