Abstract Submitted
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Self-consistent calculation of Hubbard U parameters within linear-scaling DFT GLENN MOYNIHAN, School of Physics, CRANN and AMBER, Trinity College Dublin, GILBERTO TEOBALDI, Stephenson Institute, University of Liverpool, DAVID D. O'REGAN, School of Physics, CRANN and AMBER, Trinity College Dublin — DFT+U has proven to be a computationally efficient method for correcting for the underestimation of electron localization effects, or for the absent derivative discontinuity, inherent in conventional density functionals. Invoking an approximate interpretation of DFT+U as a corrective penalty functional for the spurious curvature of the total-energy with respect to subspace occupancy, the Hubbard U parameter may be calculated [1,2], in which case DFT+U may be considered to be fully first-principles approach. We describe our approach for computing the Hubbard U and Hunds J parameters within ONETEP, a linear-scaling DFT code which comprises a complete DFT+U+J [3] implementation including ionic forces and a flexible choice of population analyses [4,5]. We discuss issues of charge preservation and self-consistency, and we demonstrate the capability of our method by means of numerical tests on the ground-state properties of selected molecules that present challenges for approximate DFT. [1] W. E. Pickett, et al., Phys. Rev. B, 58, 1201 (1998). [2] H. J. Kulik, et al., Phys. Rev. Lett. 97, 103001 (2006). [3] B. Himmetoglu, et al., Phys. Rev. B 84, 115108 (2011). [4] D. D. ORegan, et al., Phys. Rev. B 85, 085107 (2012). [5] D. D. ORegan, et al., Phys. Rev. B 83, 245124 (2011).

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