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TDDFT+ U for transition-metal complexes XIAOFENG QIAN, DAVIDE CERESOLI, ELISE LI, HEATHER J. KULIK, NICOLA MARZARI, Department of Materials Science and Engineering, MIT — Time-dependent density functional theory (TDDFT) has been used to successfully predict excited-state properties of various organic and inorganic molecular systems, such as optical absorption and circular dichroism. On the other hand, it is known that orbital-independent exchange-correlation functionals, such as LDA and GGA, tend to underestimate exchange interactions, delocalize electrons, and suffer from qualitative failures originating in self-interaction errors. In transition-metal complexes these often lead to incorrect multiplicities and charge and spin distributions already in the ground states. We implement a Hubbard-like U correction [1] to TDDFT calculations in Quantum ESPRESSO [2], using a real-time propagation scheme, and examine the effect of the Hubbard term in TDDFT predictions of optical properties. [1] H. J. Kulik, M. Cococcioni, D. A. Scherlis, and N. Marzari, Phys. Rev. Lett., 2006, 97, 103001. [2] <http://www.quantum-espresso.org/>

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