**TDDFT+ U for transition-metal complexes**

XIAOFENG QIAN, CLAUDIO 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/