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DFT+$U(\omega)$: Frequency-dependent Hubbard U correction DAVID D. O'REGAN, Trinity College Dublin, NICOLA MARZARI, Ecole Polytechnique Federale de Lausanne (EPFL) — In contemporary first-principles atomistic simulation based on DFT, the augmentation of approximate exchange-correlation functionals with spatially or energetically localized corrections, such as DFT+U, is a successful approach forimproving its applicability to strongly interacting systems. Electronic screening is a dynamical process, and since the Hubbard U parameter, in particular, is a measure of the screened Coulomb interaction, its frequency-dependent generalisation for the dynamical regime is possible. We introduce a conceptually pragmatic and computationally straightforward method, named DFT+$U(\omega)$, for calculating and incorporating strong dynamical screening effectsin spectroscopic calculations based on Kohn-Sham DFT. Our method is designedto be a minimal dynamicalextension of DFT+U, one in which computingapproximate dynamical Hubbard U functions only requires functionality that is widely available. We demonstrate our effective plasmon fitting and self-energy approximation scheme for DFT+$U(\omega)$, which enables the resulting low-energy dynamical model to be solved at the G_0W_0 level, and beyond, efficiently and effectively.

David D. O'Regan
School of Physics, Trinity College Dublin

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