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Optical spectroscopies of materials from orbital-dependent approximations ISMAILA DABO, Ecole des Ponts ParisTech, ANDREA FERRETTI, CNR Istituto Nanoscienze, MATTEO COCOCCIONI, University of Minnesota, NICOLA MARZARI, Ecole Polytechnique Federale de Lausanne — Electronic-structure calculations based upon density-functional theory (DFT) have been fruitful in diverse areas of materials science. Despite their exceptional success and widespread use, a range of spectroscopic properties fall beyond the scope of existing DFT approximations. Failures of DFT calculations in describing electronic and optical phenomena take root in the lack of piecewise linearity of approximate functionals. This known deficiency reverberates negatively on the spectroscopic description of systems involving fractionally occupied or spatially delocalized electronic states, such as donor-acceptor organic heterojunctions and heavy-metal organometallic complexes. In this talk, I will present a class of orbital-dependent density-functional theory (OD-DFT) methods that are derived from a multidensity formulation of the electronic-structure problem and that restore the piecewise linearity of the total energy via Koopmans' theorem. Such OD-DFT electronic-structure approximations are apt at describing full orbital spectra within a few tenths of an electron-volt relative to experimental photoemission spectroscopies and with the additional benefit of providing appreciably improved total energies for molecular systems with fractional occupations.

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