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Screening and linear response in Koopmans-compliant functionals NICOLA COLONNA, NGOC LINH NGUYEN, Theory and Simulations of Materials (THEOS), and National Center for Computational Design and Discovery of Novel Materials (MARVEL), EPFL, Switzerland, ANDREA FERRETTI, Centro S3, CNR Istituto Nanoscienze, I-41125 Modena, Italy, NICOLA MARZARI, Theory and Simulations of Materials (THEOS), and National Center for Computational Design and Discovery of Novel Materials (MARVEL), EPFL, Switzerland — The need to describe relaxation effects in the fractional removal or addition of an electron requires screening the orbital-dependent corrections of Koopmans-compliant functionals. Here, we present a general method to incorporate orbital-by-orbital screening based on linear-response theory. We illustrate the importance of such generalization when dealing with challenging system containing orbitals with very different chemical character, such as transition-metal complexes. Results for ionization potentials, when compared with many-body perturbation theory (MBPT) and experiments, show a remarkably good performance, comparable to the most accurate MBPT approach (G0W0@PBE0).

Nicola Colonna
THEOS, MARVEL, EPFL

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