Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Koopmans-compliant functionals as spectral theories: molecules, solids, and liquids NICOLA MARZARI, NGOC LINH NGUYEN, NICOLA COLONNA, THEOS, EPFL, ANDREA FERRETTI, S3 Center, Istituto Nanoscienze, CNR, Modena, Italy — Koopmans-compliant functionals[1] enforce a generalized criterion of piecewise linearity with respect to the fractional removal or addition of an electron (i.e. a charged excitation) from any orbital in local or semi-local total-energy DFT functionals. By doing so they lead to beyond-DFT orbital-density dependent functionals that are able to deliver spectroscopic properties. We'll present an overview of the current status when applied to ionization potentials, electron affinities, photoemission spectra, and band gaps of molecules, solids, and liquids, with results that are comparable or slightly superior to many-body perturbation theory, but with functionals that rely only on the physics of the PBE generalized-gradient approximation.

[1]I. Dabo, M. Cococcioni, and N. Marzari, arXiv:0901.2637 (2009); I. Dabo *et al.* Phys. Rev. B 82 115121 (2010).

Nicola Marzari
THEOS, EPFL

Date submitted: 15 Nov 2016 Electronic form version 1.4