Contribution ID: **137** Type: **Talk**

【502】Koopmans-compliant functionals: A reliable and efficient tool for the prediction of spectroscopic

Wednesday 29 August 2018 17:00 (15 minutes)

Approximate density functionals produce total energies that do not exhibit the expected piecewise-linear behavior as a function of the particle number, leading to a discrepancy between total and partial electron removal/addition energies and poor predictive capabilities of ionization potentials. Koopmans-compliant functional enforce a generalized criterion of piecewise linearity in the energy of any density functional with respect to the partial removal/addition of an electron from/to any orbital of the system. Koopmans'corrections to approximate density functionals, lead to orbital-density dependent potentials able to deliver accurate spectroscopic properties. Ionization potentials of a large set of molecules, photoemission spectra of organic donors and acceptors and band gaps of 35 semiconductors and insulators are presented, showing excellent agreement with experiment or higher-order theories.

Primary authors: Dr COLONNA, Nicola (EPFL); Dr NGUYEN, Ngoc Linh (EPFL); Dr FERRETTI, Andrea (CNR-Istituto Nanoscienze); Prof. MARZARI, Nicola (EPFL)

Presenter: Dr COLONNA, Nicola (EPFL)

Session Classification: Advanced Electronic-Structure Developments and Applications

Track Classification: Advanced Electronic-Structure Developments and Applications