Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Efficient Density Functional Approximation for Electronic Properties of Conjugated Systems[1] MARíLIA J. CALDAS, JOSÉ MAXIMIANO PINHEIRO JR, Institute of Physics, University of São Paulo, São Paulo, Brazil, VOLKER BLUM, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany; Duke University, Durham, NC, USA, PATRICK RINKE, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — There is on-going discussion about reliable prediction of electronic properties of conjugated oligomers and polymers, such as ionization potential IP and energy gap. Several exchange-correlation (XC) functionals are being used by the density functional theory community, with different success for different properties. In this work we follow a recent proposal [1]: a fraction α of exact exchange is added to the semi-local PBE XC [2] aiming consistency, for a given property, with the results obtained by many-body perturbation theory within the G0W0 approximation. We focus the IP, taken as the negative of the highest occupied molecular orbital energy. We choose α from a study of the prototype family trans-acetylene, and apply this same α to a set of oligomers for which there is experimental data available (acenes, phenylenes and others). Our results indicate we can have excellent estimates, within 0,2eV mean ave. dev. from the experimental values, better than through complete $E_{N-1} - E_N$ calculations from the starting PBE functional. We also obtain good estimates for the electrical gap and orbital energies close to the band edge.

[1] V. Atalla, M. Yoon, F. Caruso, P. Rinke, M. Scheffler PRB 88, 165122 (2013).
[2] J.P. Perdew, K. Burke, M. Ernzerhof PRL 77, 3865 (1996).

[1]Work supported by FAPESP, CNPq, and CAPES, Brazil, and DAAD, Germany

Marília J. Caldas
Institute of Physics, University of São Paulo, Brazil

Date submitted: 15 Nov 2013 Electronic form version 1.4