Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Reliability of the Tran-Blaha functional in predicting band gaps and widths GIAN-MARCO RIGNANESE, WAROQUIERS DAVID, AURÉLIEN LHERBIER, ANNA MIGLIO, MARTIN STANKOVSKI, SAMUEL PONCE, Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, MICAEL OLIVEIRA, Center for Computational Physics, University of Coimbra, Portugal, MATTEO GIANTOMASSI, XAVIER GONZE, Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain — For a set of oxides and semiconductors, we compute the electronic band structures (gaps and widths) within Density-Functional theory (DFT) using the Tran-Blaha (TB09) functional [Phys. Rev. Lett. **102**, 226401 (2009)]. We compare them with those obtained from (i) DFT using the local-density approximation (LDA), (ii) many-body perturbation theory (MBPT), and (iii) experiments. TB09 leads to band gaps in much better agreement with experiment than the LDA. However, the valence (and conduction) band widths are often underestimated (noticeably more than in LDA). MBPT corrections are obtained peforming one-shot *GW* calculations using DFT eigenenergies and wavefunctions as starting point (both LDA and TB09 are considered). These corrections lead to a much better agreement with experimental data for the band widths. The MBPT band gaps obtained starting TB09 are close to those from quasi-particle self-consistent *GW* calculations, at a much reduced cost. Finally, we explore the possibility to tune a semi-empirical parameter present in the TB09 functional aiming to obtain simultaneously better gaps and band widths. We find that these requirements are conflicting.

Gian-Marco Rignanese
Institute of Condensed Matter and Nanosciences,
Université Catholique de Louvain

Date submitted: 11 Dec 2012 Electronic form version 1.4