Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Efficient computation of GW energy level corrections for molecules described in a plane wave basis BRUNO ROUSSEAU, JONATHAN LAFLAMME JANSSEN, MICHEL CÔTÉ, University of Montreal — An efficient computational approach is presented to compute the ionisation energy and quasi-particle band gap at the level of the GW approximation when the Hilbert space is described in terms of plane waves. The method relies on ab initio calculations as a starting point. Then, the use of the Sternheimer equation eliminates slowly convergent sums on conduction states. Further, the Lanczos method is used to efficiently extract the most important eigenstates of the dielectric operator. This approach avoids the explicit computation of matrix elements of the dielectric operator in the plane wave basis, a crippling bottleneck of the brute force approach. The method is initially applied to organic molecules of current interest in the field of organic photovoltaics. Given the completeness of the plane wave basis, systematic convergence studies can be conducted. Furthermore, the method can readily be extended to describe polymers, which are also of interest for photovoltaic applications, but remain a significant computational challenge for methods based on localized basis sets.

Bruno Rousseau
University of Montreal

Date submitted: 17 Nov 2012 Electronic form version 1.4