VIENNA COMPUTATIONAL MATERIALS LABORATORY
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AB INITIO MANY BODY THEORY AND CALCULATIONS OF ELECTRONIC EXCITATIONS, SPECTROSCOPY AND QUANTUM TRANSPORT.

A TALK BY DR. PAOLO E. TREVISANUTTO,
NATIONAL NANOTECHNOLOGY LABORATORY OF THE CONSIGLIO NAZIONALE DELLE RICERCHE IN LECCE, ITALY

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Ab initio GW approximation (GWA) calculations have been widely used to provide the quasi particle band structure of semiconductors, large-gap insulators, metals [1].
GWA is also defined as a dynamically screened Hartree-Fock (HFA) approximation where the bare Coulomb potential v in the HFA self energy is replaced by a dynamically screened potential W.
The electron-electron correlation in the screened potential W is set by long range charge-density ("plasmons") oscillation which makes the GWA be suitable for solids with delocalised s and p orbitals (called "weakly correlated systems"). Static approximation to GWA self energy is a sum of Screened Exchange potential plus a Coulomb Hole (Cohsex approximation). Recently, self-consistent (SC) GWA and Cohsex calculations have been performed to describe some systems considered strongly correlated [2].
The optical spectrum where the hole-electron interactions play a role, is obtained by solving the Bethe Salpeter equation (BSE).
We present ab initio many-body GWA and BSE calculations of the electronic excitations in graphene as compared to graphite [3, 4]. We further discuss the results of ab initio GWA calculations in the Landauer approach for the Quantum Transport problem [5].
Finally, we propose a functional based on Cohsex for the Reduced Density Matrix Functional Theory (reduced density matrix extension of the Density Functional Theory).

[1] F. Aryasetiawan and F. Gunnarson Rep. Prog. Phys. 61, 237 (1998)
[2] M. Gatti et al. Phys. Rev. Lett 99, 266402 (2007)
[3] P.E.Trevisanutto et al. Phys. Rev. Lett. 101, 226405 (2008)
[4] P.E. Trevisanutto et al. Phys. Rev. B 81, 121405(R) (2010)
[5] T. Rangel et al. Phys. Rev. B 84, 045426 (2011)