GW renormalization of the electron–phonon coupling

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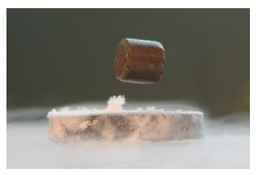
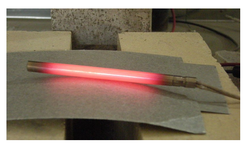
Electron–phonon coupling: why?

The Electron-Phonon Coupling (EPC) is the main ingredient to describe plenty of physical phenomena

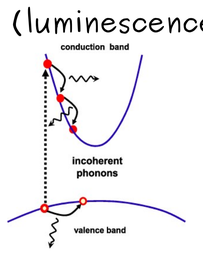
Superconductivity



Joule's heating

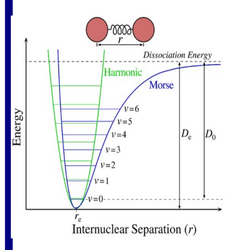


Electron relaxation (luminescence)



Raman Spectroscopy

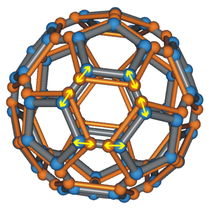
Electron–phonon coupling: definition



$$H(x+u) = H(x) + \frac{\partial H}{\partial x} u + \frac{1}{2} \frac{\partial^2 H}{\partial x^2} u^2 + \ldots$$

For every single particle Hamiltonian (Kohn-Sham, Tight-binding, etc..)

Second order expansion



LUMO (3-fold)

Stepwise deformation

EPC ~ |slope|²

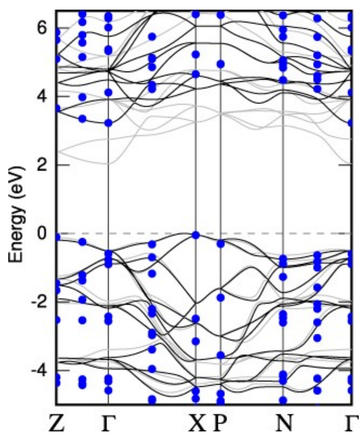
Structural deformation

Changes in electronic structure

Within the Harmonic approximation we can expand the Kohn-Sham(KS) Hamiltonian up to the second order in the atomic displacements. The EPC matrix elements are the derivatives of this Hamiltonian

Correction to the band structure

It is known that KS band structure is a poor representation of the band structure measured in experiments due to the band-gap problem, the levels order and so on...



Using Many–body Perturbation Theory we can correct KS band structure and get better agreement with the experiments

$$\epsilon_{QP} \simeq \epsilon_{KS} + \int G(\omega-\omega')W(\omega') + \ldots$$

$$W(\omega) = \frac{V_{ee}}{\epsilon(\omega)}$$

GW is the first order correction in terms of screened interaction

Aryasetiawan, F., & Gunnarsson, O. The GW method. Reports on Progress in Physics, **61**(3), 237.(1998).

It works very well !!!

Is the GW correction important also for the band-structure derivatives (the EPC matrix elements)?

Simplified approach

GW corrections to the electron-phonon coupling provide very accurate results in comparison with experiments, however these calculations are quite expensive.
Here we tested two approximations commonly used in the Bethe-Salpeter equation for the optical response in order to speed up calculations

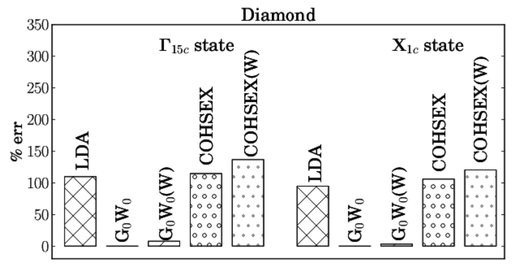
1) Static screening (COHSEX)

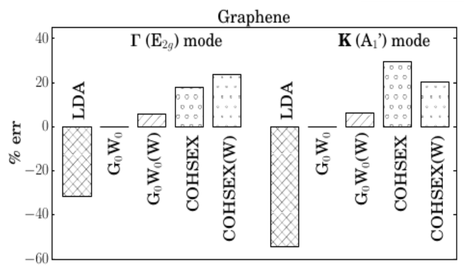
Inspired by the Bethe-Salpeter equation

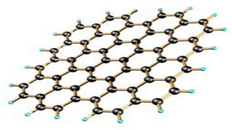
$$\frac{\partial \Sigma^{GW}}{\partial u^{q\nu}} \simeq \frac{\partial \Sigma^{COHSEX}}{\partial u^{q\nu}} \longleftrightarrow W(\omega) \simeq W(0)$$

2) Constant screening respect to the phonon displacement

$$\frac{\partial GW}{\partial u^{q\nu}} \simeq \left(\frac{\partial G}{\partial u^{q\nu}}\right) W$$







Approximation to the GW self-energy electron-phonon coupling gradients
C. Faber et al.
Physical Review B **91** (15), 155109(2015)

Conclusions

1) Electron-phonon coupling from Kohn-Sham under/overestimate the real one

2) Many-Body-Perturbation Theory can be used to correct the EPC

3) The new EPC matrix elements improve: **Raman, phonons, band-gap renomalization, T_c**

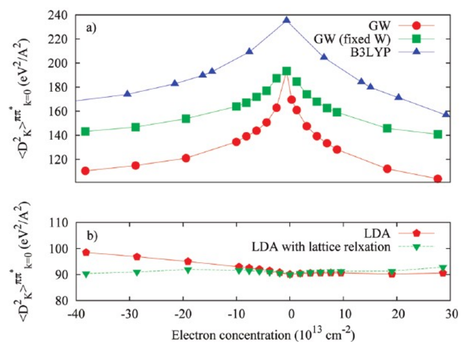
4) **New physics can appear!**

5) If calculations are too heavy …. use our **simplified approach**

Approximation to the GW self-energy electron-phonon coupling gradients
C. Faber et al. PRB **91** (15), 155109(2015)

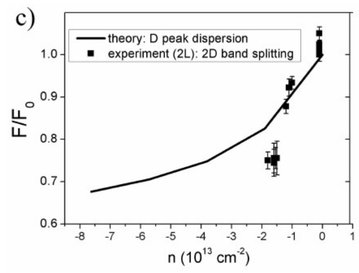
New physics appears…

GW corrections not only modify the size of EPC in graphene but also its behavior with doping.
We predicted this effect in 2010 and then two independent experiments verified this finding

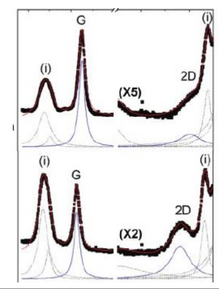


EPC for the K-A' phonon aquires a strong doping dependence

Doped graphene as tunable electron-phonon coupling material
C. Attaccalite et al., Nanoletters, **10**, 1172(2010)

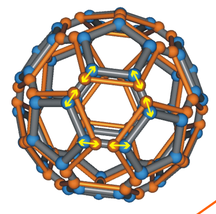


Raman signature of electron-electron correlation in chemically doped few-layer graphene
Phys. Rev. B **83**, 241401(R) (2011)
Matteo Bruna and Stefano Borini

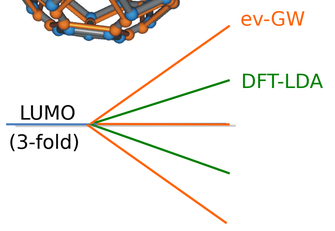


Pressure-mediated doping in graphene
Nanoletters, **11**, 3564 (2011)
J. Nicolle,D. Machon, P. Poncharal,O. Pierre-Louis and Alfonso San-Miguel

EPC in molecules



EPC in fullerene compared in LDA and evGW compared with the value obtained from exp.



Electron-phonon potential

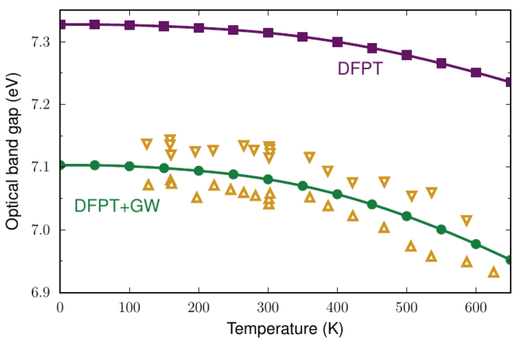
LDA	73 meV
evGW	101 meV
Exp.	107 meV

DFT: J. Laflamme-Janssen, PRB 2010;
GW: C. Faber, J. of Mat. S., **47**, 7472(2012)
Exp: Wang, JCP 2005; Hands, PRB 2008;

Electron–phonon coupling and charge-transfer excitations in organic systems from many-body perturbation theory
C. Faber et al., J. of Material Science, **47**, 7472(2012)

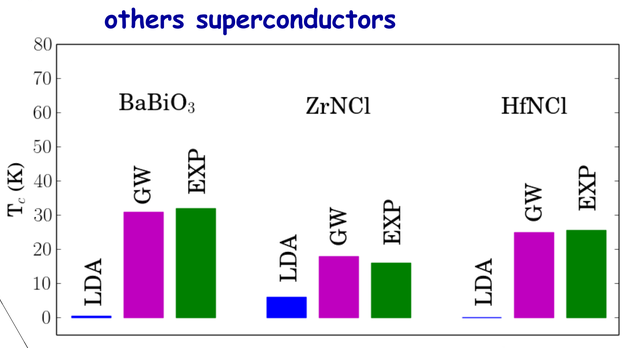
Diamond and superconductors

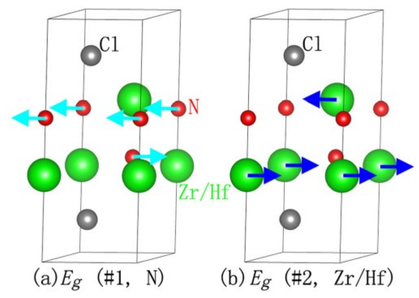
Diamond gap versus temperature



G. Antonius et al.
PRL **112**, 215501 (2014)

Critical temperature Tc in Bismuthates, Chloronitrides and others superconductors

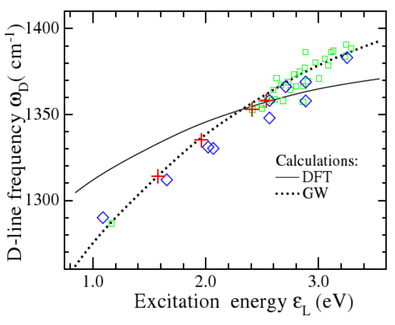




Z. P. Yin, A. Kutepov, and G. Kotliar
Phys. Rev. X **3**, 021011 (2013)

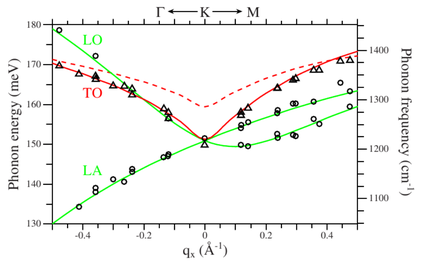
EPC in graphene

First calculation with GW correction for the EPC



Raman D-line dispersion in graphene

M. Lazzeri,et al.
PRB **78**, 081406(R) (2008)



Phonon dispersions around the K point of graphite by inelastic x-ray scattering

$\langle D_K^2 \rangle_F = 166 (eV/\mathring{A})$ inelastic x-ray

$\langle D_K^2 \rangle_F = 164 (eV/\mathring{A})$ GW

A. Grüneis et al . Phys. Rev. B **80**, 085423 (2009)