Non Equilibrium dynamics Models and Excited state properties of low-dimensional SYStems (NEMESYS)

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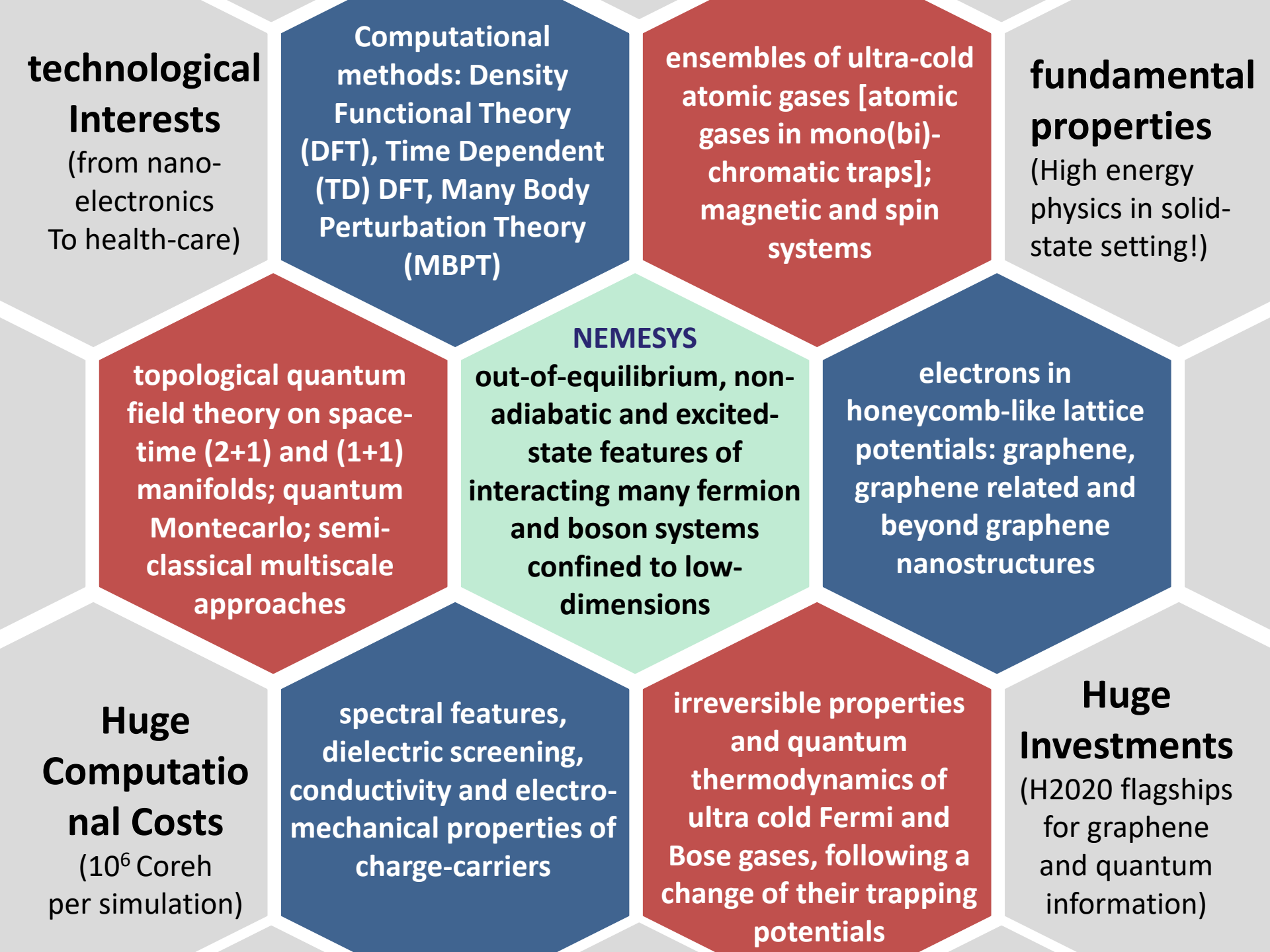
UNIVERSITÀ DEGLI STUDI DI BARI ALDO MORO

XVII workshop on Statistical Mechanics and non Perturbative Field Theory
Bari (15.12.2017)


technological Interests
(from nano-electronics To health-care)
Computational methods: Density Functional Theory (DFT), Time Dependent (TD) DFT, Many Body Perturbation Theory (MBPT)
ensembles of ultra-cold atomic gases [atomic gases in mono(bi)-chromatic traps]; magnetic and spin systems
fundamental properties
(High energy physics in solid-state setting!)
topological quantum field theory on space-time (2+1) and (1+1) manifolds; quantum Montecarlo; semi-classical multiscale approaches
NEMESYS
out-of-equilibrium, non-adiabatic and excited-state features of interacting many fermion and boson systems confined to low-dimensions
electrons in honeycomb-like lattice potentials: graphene, graphene related and beyond graphene nanostructures
Huge Computational Costs
(10^6 Coreh per simulation)
spectral features, dielectric screening, conductivity and electro-mechanical properties of charge-carriers
irreversible properties and quantum thermodynamics of ultra cold Fermi and Bose gases, following a change of their trapping potentials
Huge Investments
(H2020 flagships for graphene and quantum information)

What we're good at

Parameter-free **Density Functional Theory** (DFT)

Time Dependent DFT (TDDFT)

Many Body Perturbation Theory (MBPT)

Green's Function (GF) techniques

HPC modules (abinit, cpmd, crystal14, nwchem, qe, vasp, yambo) & self-developed programs

MOST RELEVANT PUBLICATIONS in 2017

APS (2 PRL, 2 PRA, 8 PRB, 1 PR App.);

AIP (1 Appl. Phys. Lett., 1 AIP Advances);

ACS (1 Nanoletters, 1 Nanophotics);

Nature (1 Nature Communications, 1 Nature Nanotechnology, 2 Scientific Reports, 1 NPJ Quantum Information);

AAAS (1 Science)

Today's Topic

PHYSICAL REVIEW B **96**, 201408(R) (2017)

RAPID COMMUNICATIONS

DOI: 10.1103/PhysRevB.96.201408

Calibration of the fine-structure constant of graphene by time-dependent density-functional theory

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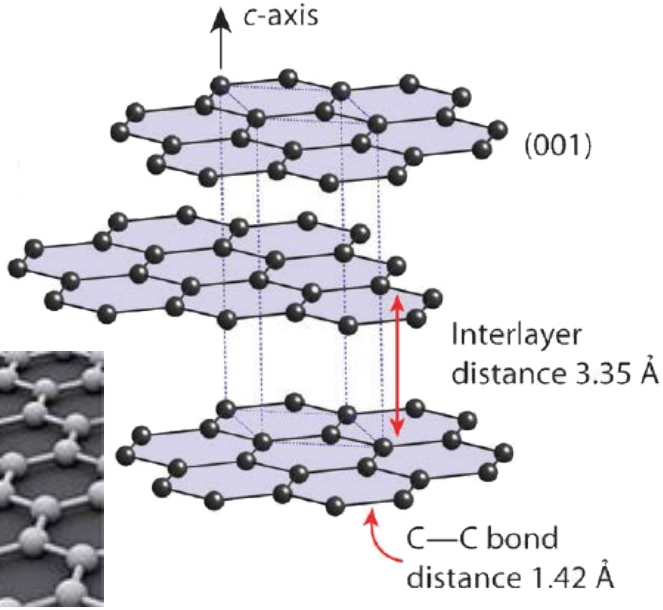
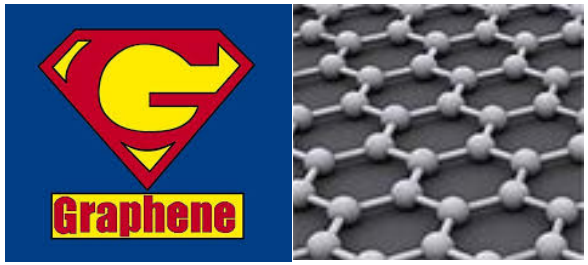
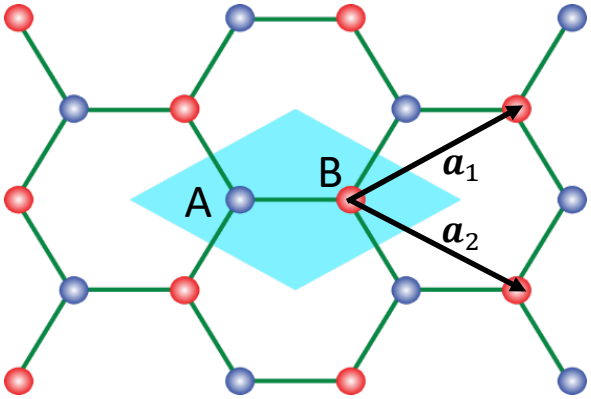
GRAPHITE vs GRAPHENE



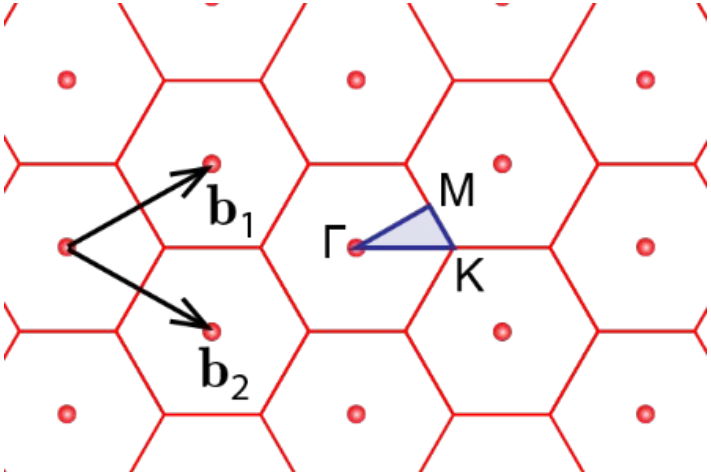


geometry (real space)



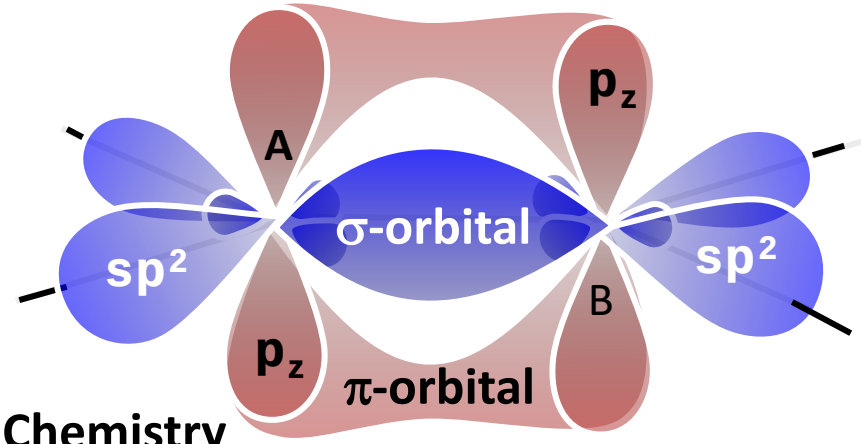
$$\boldsymbol{R} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2$$

geometry (reciprocal space)



$$\boldsymbol{G} = m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2$$

Wallace, Phys. Rev. 71, 622 (1947)
a simple exercise in quantum mechanics



Chemistry

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π states (Block's Theorem, Tight-binding approach)

$$|\pi_{\boldsymbol{k}}\rangle = a_{\boldsymbol{k}} \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} |p_z(\boldsymbol{R})\rangle + b_{\boldsymbol{k}} \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}+\boldsymbol{\delta})} |p_z(\boldsymbol{R}+\boldsymbol{\delta})\rangle$$

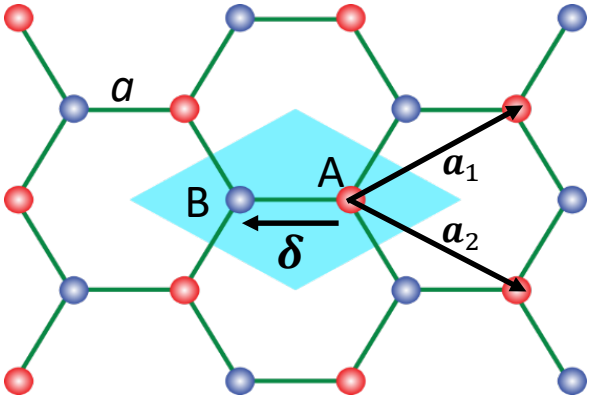
one-electron Hamiltonian H=T+V, with V translationally invariant under translations of R

minimizing $E[\pi_{\boldsymbol{k}}] = \dfrac{\langle \pi_{\boldsymbol{k}} | \hat{H} | \pi_{\boldsymbol{k}} \rangle}{\langle \pi_{\boldsymbol{k}} | \pi_{\boldsymbol{k}} \rangle}$

with respect to $\boldsymbol{a}_k$ and $\boldsymbol{b}_k$ leads to

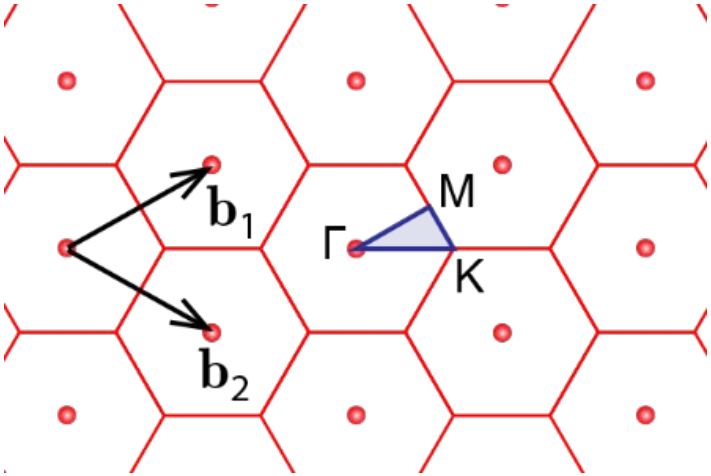
$$\left| \begin{pmatrix} E_{2p} & V_0 f_{\boldsymbol{k}} \\ V_0 f_{\boldsymbol{k}}^* & E_{2p} \end{pmatrix} - E \begin{pmatrix} 1 & S_0 f_{\boldsymbol{k}} \\ S_0 f_{\boldsymbol{k}}^* & 1 \end{pmatrix} \right| = 0$$

with $f_{\boldsymbol{k}} = e^{-iak_x} + 2\, e^{\frac{iak_x}{2}} \cos\dfrac{\sqrt{3}ak_y}{2}$



real space

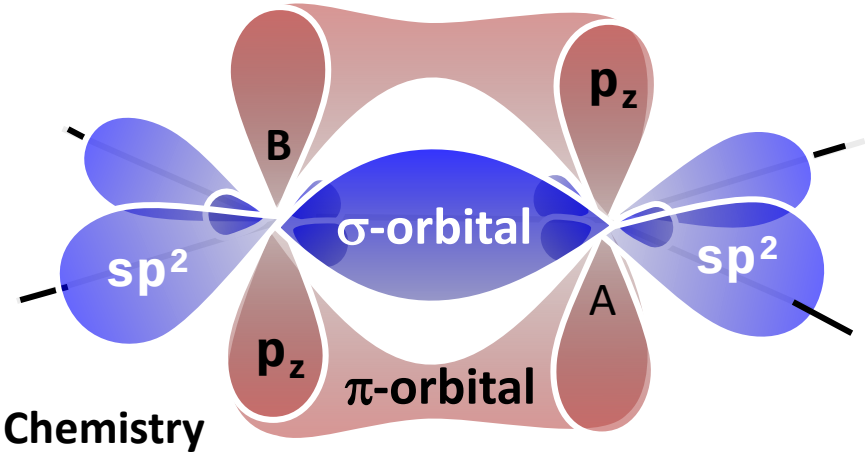
$$\boldsymbol{R} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2$$



reciprocal space

$$\boldsymbol{G} = m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2$$

Wallace, Phys. Rev. 71, 622 (1947)



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with $f_k = e^{-iak_x} + 2\,e^{\frac{iak_x}{2}}\cos\dfrac{\sqrt{3}ak_y}{2}$

$S_0 = \langle p_z(R)|p_z(R+\delta)\rangle \sim 0.1$

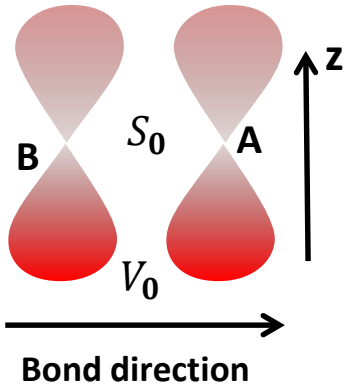
and

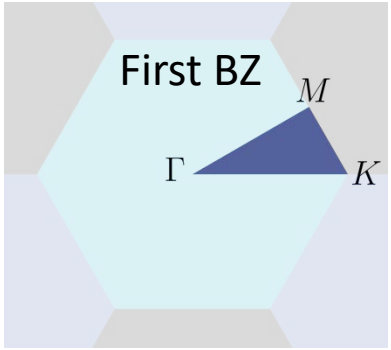
$V_0 = \langle p_z(R)|\hat{V}|p_z(R+\delta)\rangle \sim 3.2$ eV

Then, assuming E_{2p}=0, we get:

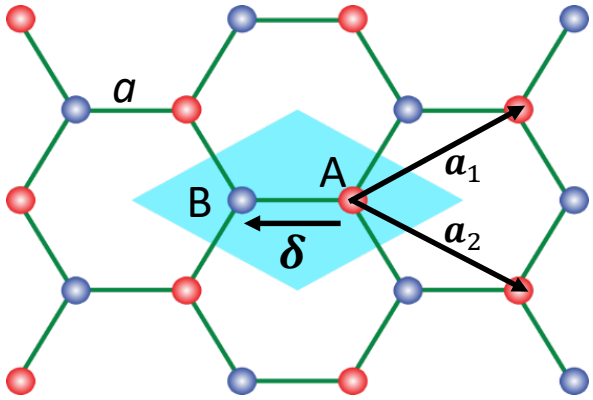
$$\varepsilon_\pi(k) = \frac{V_0|f_k|^2}{1+S_0|f_k|^2}$$

$$\varepsilon_{\pi^*}(k) = \frac{-V_0|f_k|^2}{1-S_0|f_k|^2}$$



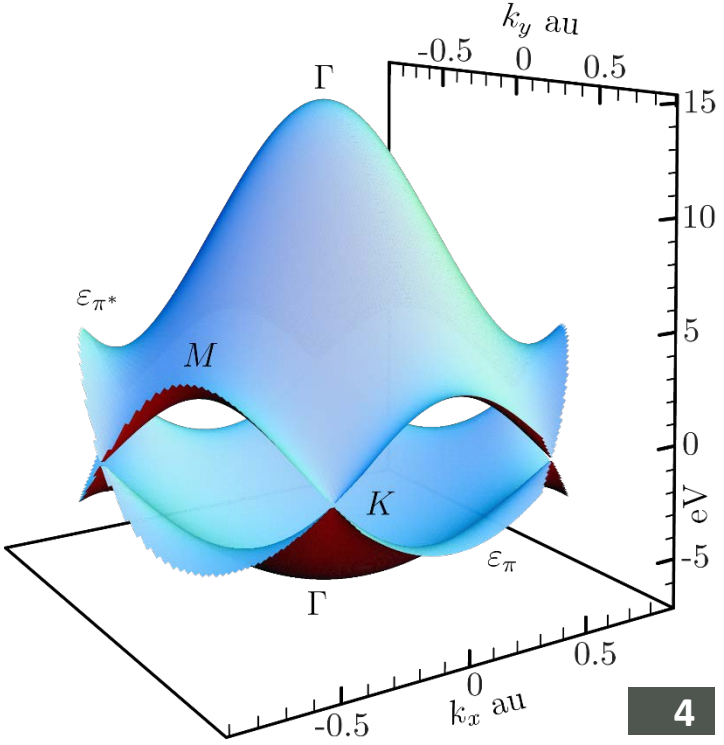


k-space



real space

Wallace, Phys. Rev. 71, 622 (1947)



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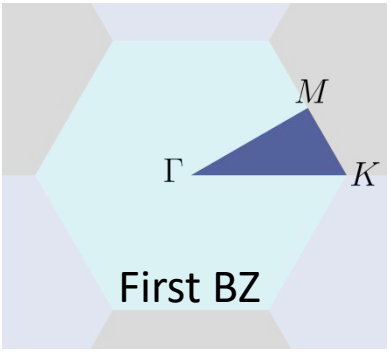
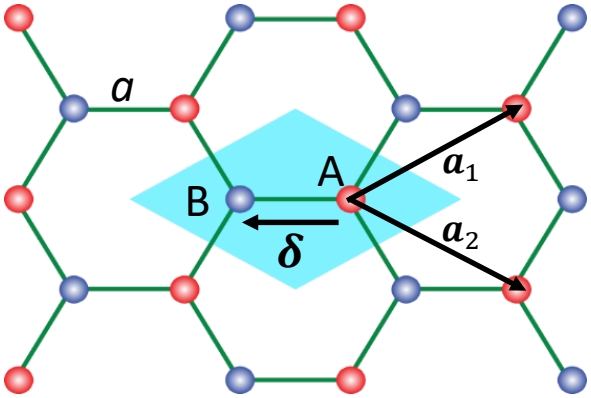
with respect to a_k and b_k leads to

$$\left|\begin{pmatrix} E_{2p} & V_0 f_k \\ V_0 f_k^* & E_{2p} \end{pmatrix} - E\begin{pmatrix} 1 & S_0 f_k \\ S_0 f_k^* & 1 \end{pmatrix}\right| = 0$$





with $f_k = e^{-iak_x} + 2\,e^{\frac{iak_x}{2}}\cos\dfrac{\sqrt{3}ak_y}{2}$

$S_0 = \langle p_z(R)|p_z(R+\delta)\rangle \sim 0.1$

and

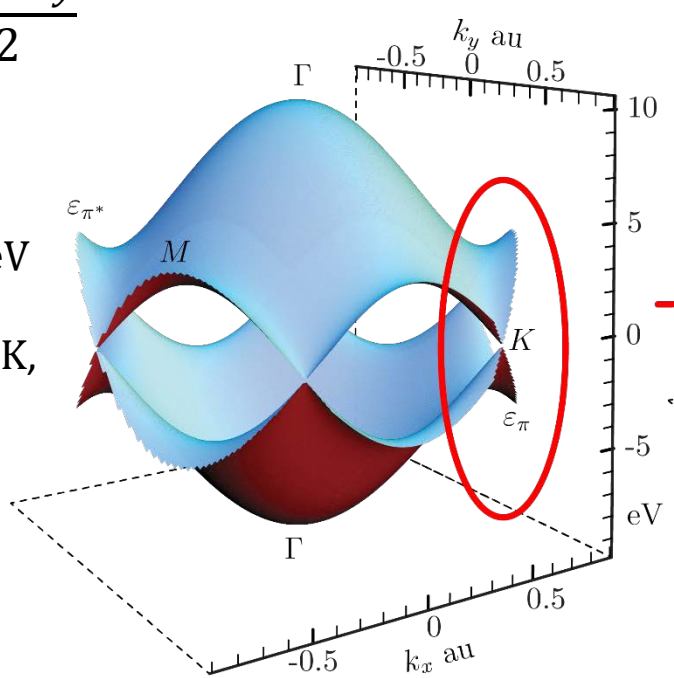
$V_0 = \langle p_z(R)|\hat{V}|p_z(R+\delta)\rangle \sim 3.2$ eV

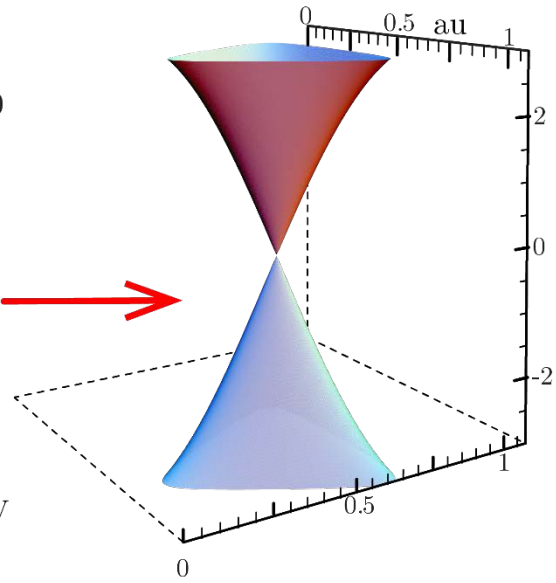
Then, assuming E_{2p}=0 and letting $k \to$ K, we get:

$$\varepsilon_\pi(k) \approx -\hbar v_F\,|k-\mathrm{K}|$$

$$\varepsilon_{\pi^*}(k) \approx \hbar v_F\,|k-\mathrm{K}|$$

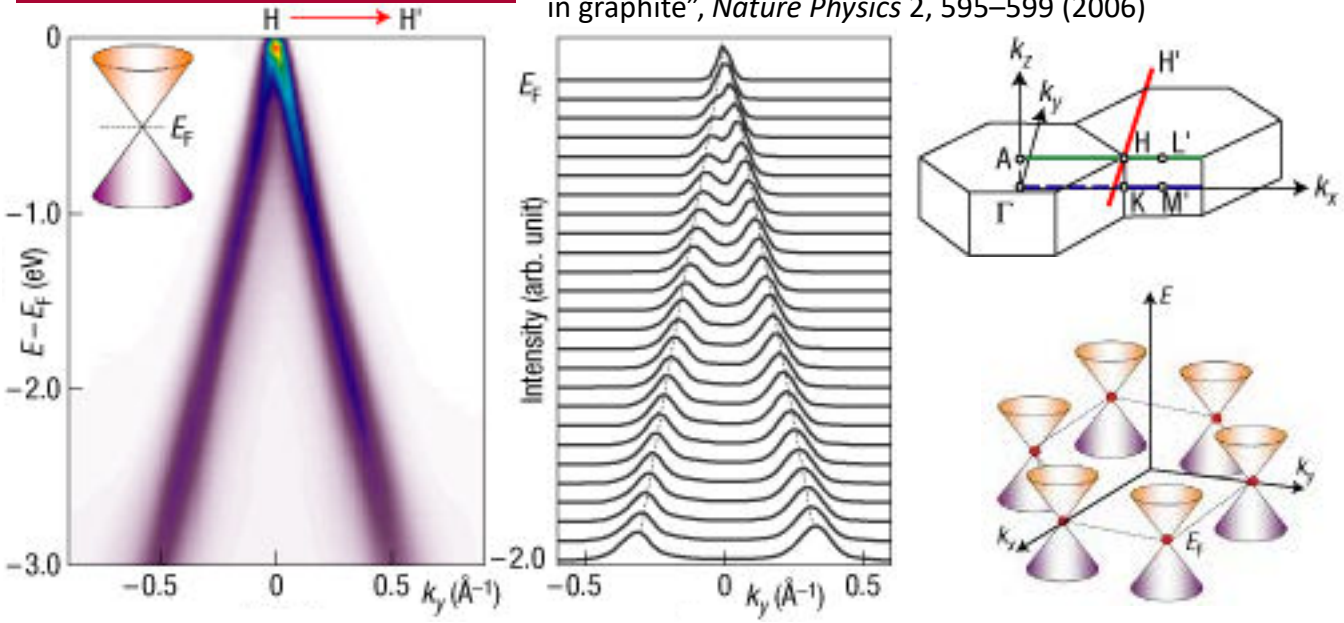
Wallace, Phys. Rev. 71, 622 (1947)



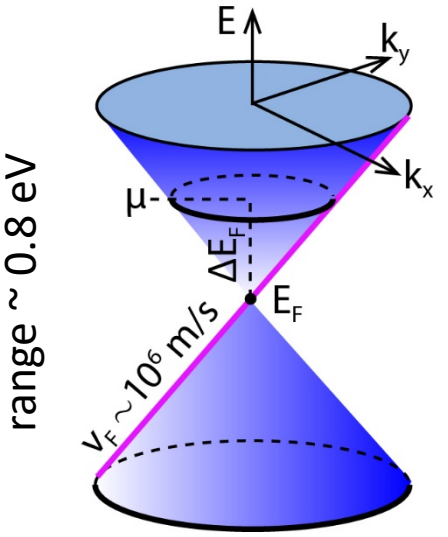


Massless Dirac Fermions

S. Y. Zhou et al., "First direct observation of Dirac fermions in graphite", *Nature Physics* 2, 595–599 (2006)



Dirac Cone (Positive Doping)



$$\omega(k) = v_F\,|\boldsymbol{k}| \qquad v_F \sim c/300$$

Interaction with light

QED

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \xrightarrow{e=\hbar=\frac{1}{4\pi\epsilon_0}=1} \frac{1}{c} \sim \frac{1}{137}$$

Graphene

$$\alpha_g = \frac{e^2}{4\pi\epsilon_0\hbar v_F} \overset{\text{au}}{\Rightarrow} \frac{1}{v_F} \sim 2.2!$$

Dressed interaction

The bare fine-structure constant of graphene is too large for any perturbation treatments and too small for close coupling approaches!!

$$\alpha_g^*(\boldsymbol{q},\omega) = \frac{e^2}{4\pi\hbar\epsilon_0 v_F}\langle\epsilon_r^{-1}\rangle(\boldsymbol{q},\omega) \overset{\text{au}}{\Rightarrow} \frac{1}{v_F}\langle\epsilon_r^{-1}\rangle(\boldsymbol{q},\omega)$$

Static limiting value

$$\tilde{\alpha}_g = \alpha_g^*(\boldsymbol{0},0)$$

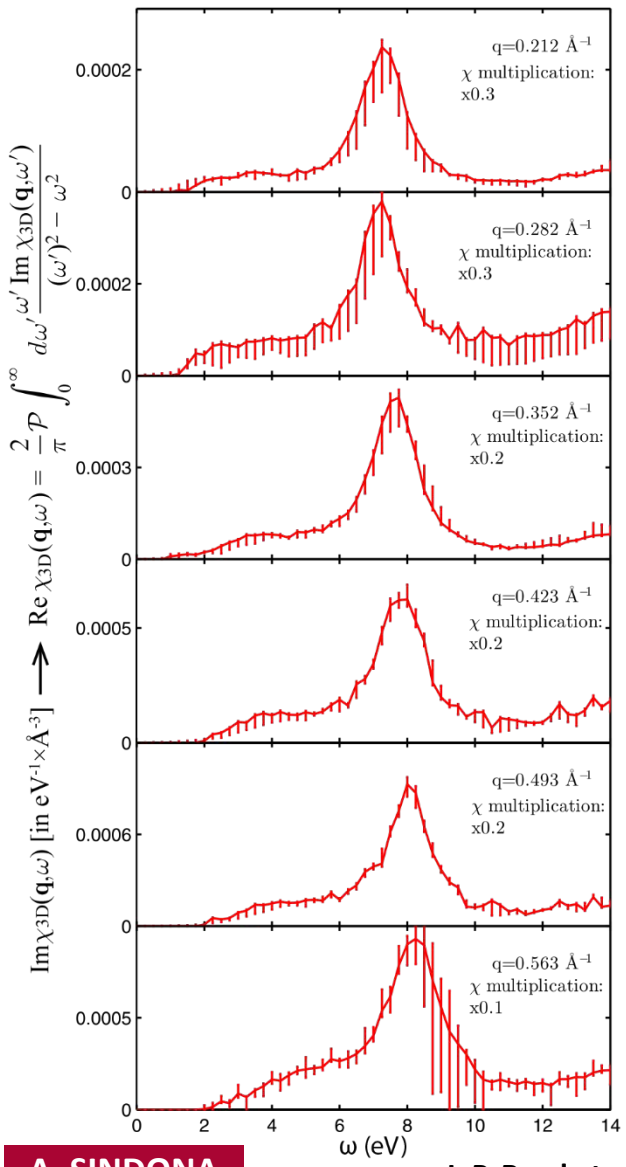
A more complete 'view' of the interaction strength amounts to replacing the vacuum permittivity with the dynamic permittivity, obtained by transferring an energy ω and a momentum q to the system

How to measure α in graphene?

$$V_{2D}(q) = \frac{2\pi}{q} \quad V_{3D}(q) = V_{2D}(q)F_d(q)$$

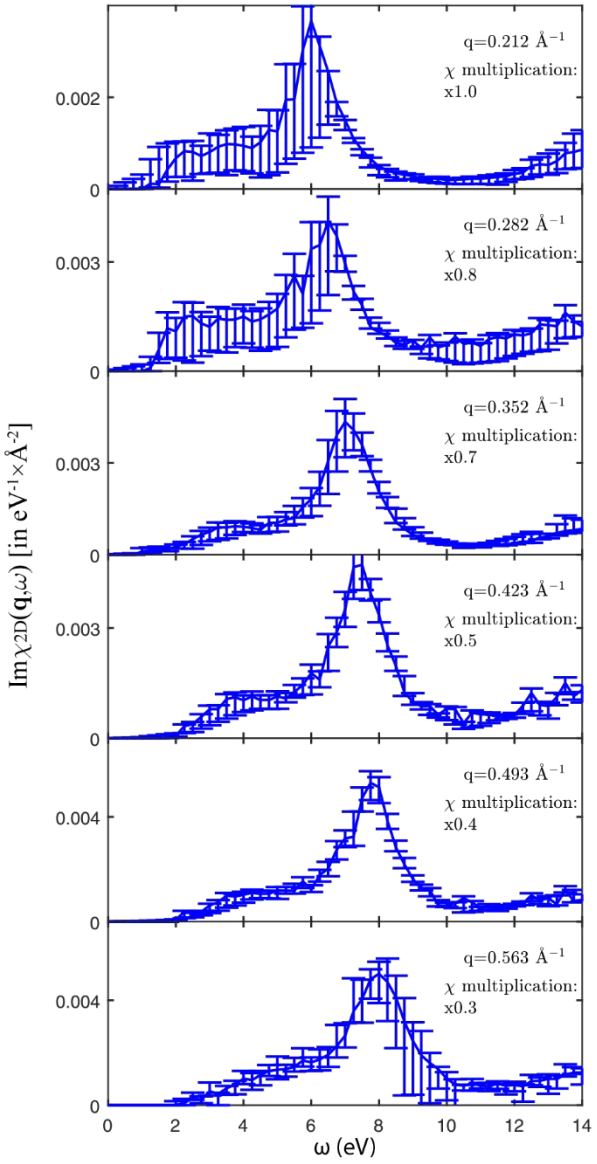
inelastic x-ray scattering (IXS) experiments on graphite:

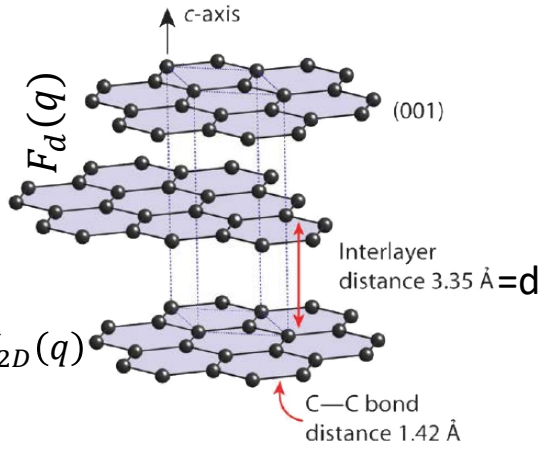
measured intensity $\propto -\frac{1}{\pi}\frac{1}{1-e^{-\beta\hbar\omega}}\,\mathrm{Im}\,\chi_{3D}(\mathbf{q},\omega)$



reconstruction of the imaginary susceptibility of graphene:

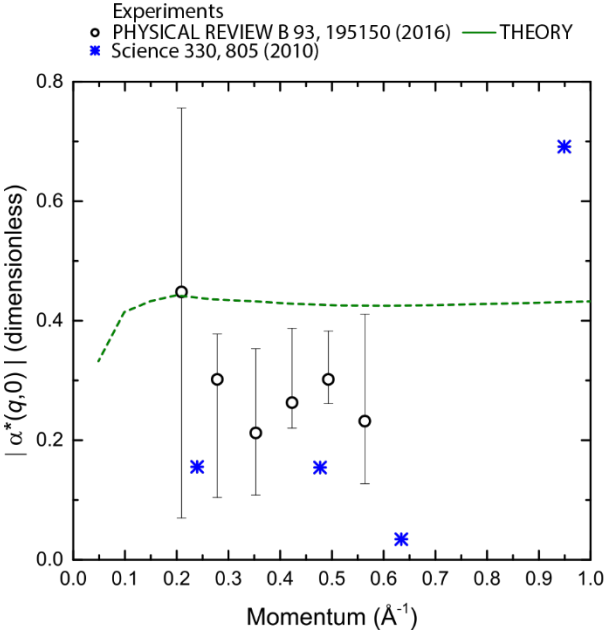
$$\chi_{2D}(\mathbf{q},\omega) = \frac{\chi_{3D}(\mathbf{q},\omega)}{1-[V_{2D}(\mathbf{q})d - V_{3D}(\mathbf{q})]\chi_{3D}(\mathbf{q},\omega)}\,d$$





Reconstruction of the dressed fine-structure constant

$$\alpha_g^*(\mathbf{q},\omega) = \frac{\alpha}{\epsilon_{2D}} = \alpha_g\,[1 + V_{2D}(\mathbf{q})\chi_{2D}(\mathbf{q},\omega)]$$



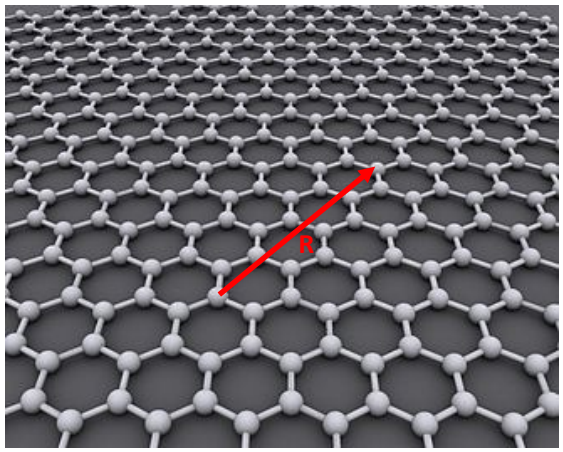
J. P. Reed et al, Science 330, 805 (2010) & Yu Gan et al, Phys. Rev. B 93, 195150 (2016)

Ab initio calculation of α in graphene

Ground-state properties (Density Functional Theory)

`Available on Marconi: abinit,qe,vasp`

Stationary Schrödinger Equation ($e = m_e = \hbar = 1$)



$$H\,\Psi = \left[\sum_i^N \frac{-\nabla_i^2}{2} + \sum_i^N \sum_{\boldsymbol{R}} \frac{-Z}{|\boldsymbol{r}_i - \boldsymbol{R}|} + \frac{1}{2}\sum_{i\neq j}^N \frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}\right]\Psi = E\,\Psi$$

Kohn-Sham DFT for electrons

Variational Principle

$$\min_{\Psi} \langle \Psi | \hat{H} | \Psi \rangle = E_0[n]$$

Self-Consistent KS Equations

$$\left[\frac{-\hbar^2\nabla^2}{2m} + V_{KS}[n]\right]\psi_i = \varepsilon_i \psi_i$$

LDA

$$n(\boldsymbol{r}) = \sum_{i\ \mathrm{occ}} |\psi_i(\boldsymbol{r})|^2 \longrightarrow V_{KS}[n] = \sum_{\boldsymbol{R}} \frac{-Z}{|\boldsymbol{r} - \boldsymbol{R}|} + \int d^3r' \frac{n(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} + \frac{\delta \mathrm{E_{xc}}}{\delta n(\boldsymbol{r})}$$

The ground state properties are uniquely determined from the electron density

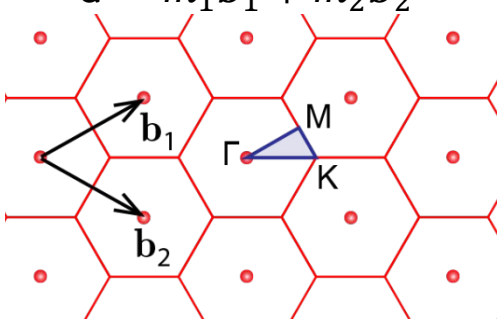
PW-DFT

$i = (\nu, \boldsymbol{k})$

$$\psi_{\nu\boldsymbol{k}}(\boldsymbol{r}) = \sum_{\boldsymbol{G}} \frac{c_{\nu\boldsymbol{k}+\boldsymbol{G}}}{\sqrt{\Omega}} e^{i(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{r}}$$

$$\boldsymbol{G} = m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2$$

Reciprocal Lattice



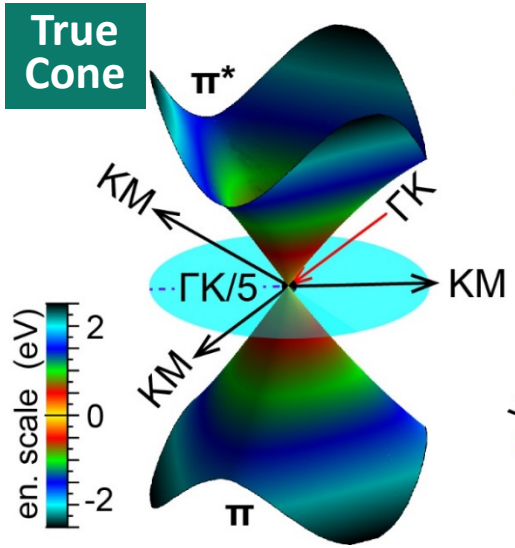
$$\frac{|\boldsymbol{k}+\boldsymbol{G}|^2}{2} < 50\ \mathrm{eV}$$

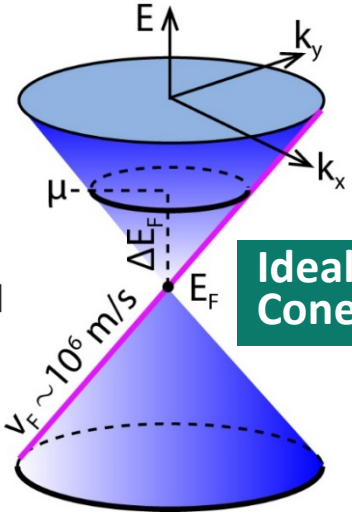
$\boldsymbol{k} \in \Gamma KM$ + 12 symm.

1-10⁵ core h depending on the resolution

10⁴-10⁵ coefficients $c_{\nu\boldsymbol{k}+\boldsymbol{G}}$ per wave function

True Cone

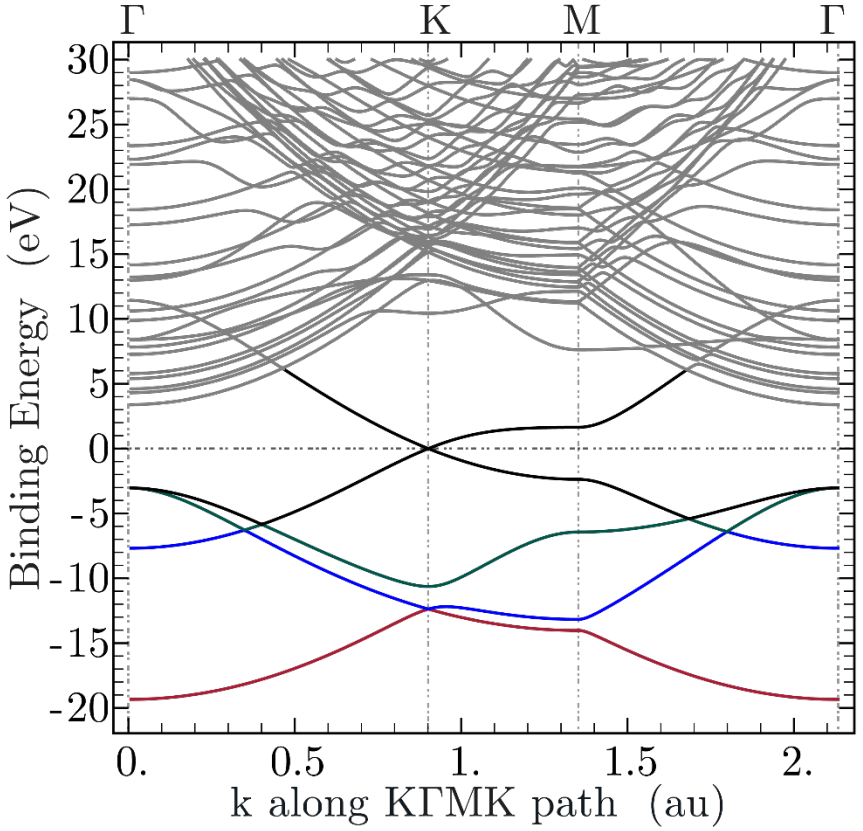


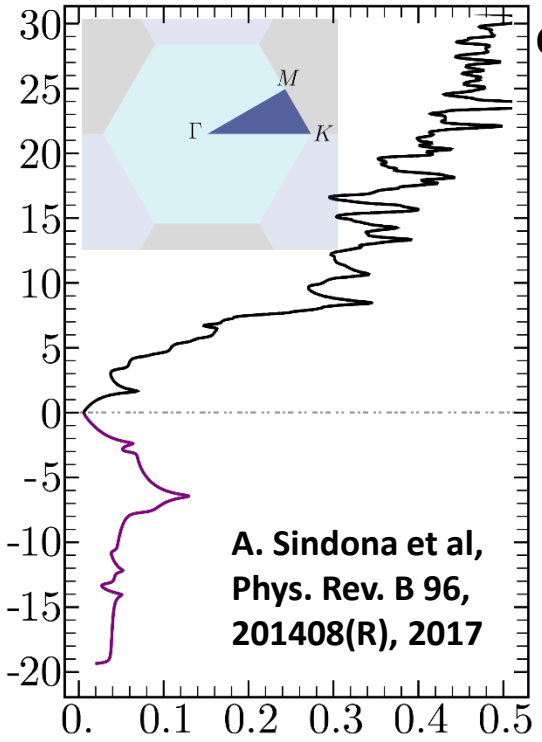


Ideal Cone

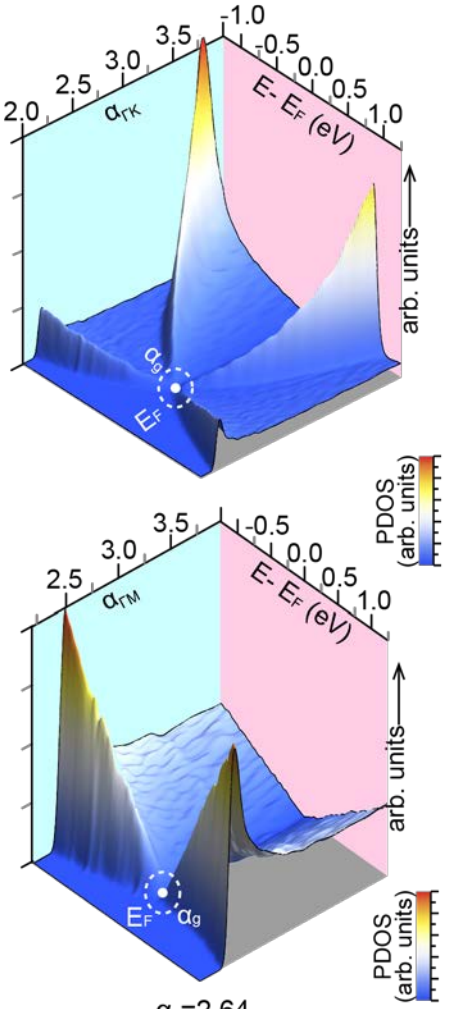
Ab initio calculation of α in graphene

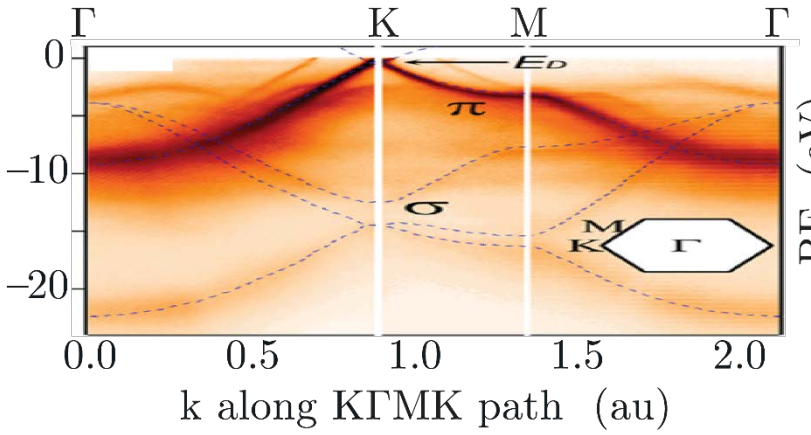
Full Band Structure (PW-DFT)



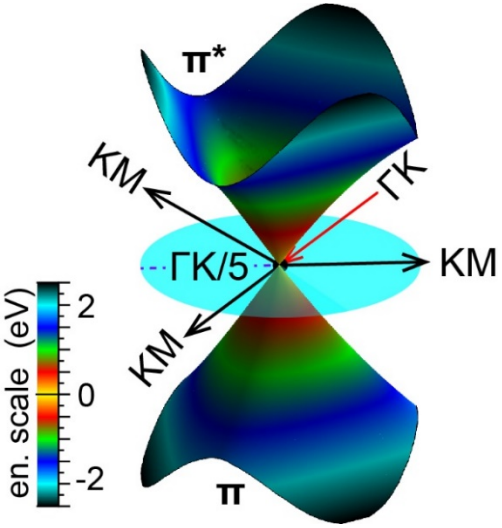


Static fine-structure Constant (Dirac Fermions)





Bostwick et al, Nature Physics 3, 36 - 40 (2007)



Ab initio calculation of α in graphene

A. Sindona et al, "Fundamental and applied Electromagnets", Springer 2016

Time-Dependent DFT (self-developed MPI codes)

The NEMESYS Project
UNICAL-LNF-ToV-TIFFPA

INFN Istituto Nazionale di Fisica Nucleare

PW-DFT

Eigenvectors

$$\psi_{\nu \boldsymbol{k}}(\boldsymbol{r}) = \sum_{\boldsymbol{G}} \frac{c_{\nu \boldsymbol{k}+\boldsymbol{G}}}{\sqrt{\Omega}} e^{i(\boldsymbol{k}+\boldsymbol{G})\cdot \boldsymbol{r}}$$

ν band index
k wave vector in IrrBZ

Eigenvalues $\varepsilon_{\nu \boldsymbol{k}}$

Self-Consistent KS Potential

$$V_{KS}(\boldsymbol{r}) = V_{ext}(\boldsymbol{r}) + V_H[n](\boldsymbol{r}) + V_{XC}[n](\boldsymbol{r})$$

Electron Density

$$n(\boldsymbol{r}) = \sum_{\nu \boldsymbol{k} \in \mathrm{IrrBZ}}^{occ} w_{\boldsymbol{k}} |\psi_{\nu \boldsymbol{k}}(\boldsymbol{r})|^2$$

Linear Response Theory

Small perturbation

$$\delta V_{\mathrm{ext}} \rightarrow \delta V_{KS} \rightarrow \delta n = \chi_0 \delta V_{KS}$$

Unperturbed density-density response

$$\chi_0^{\pm}(\boldsymbol{r}, \boldsymbol{r}'; t) = \mp \frac{i}{\hbar} \lim_{\eta \to 0} \langle [n_I(r,t), n(r')] \rangle \, e^{\mp \frac{\eta t}{\hbar}},$$

Extra electron or incident photon $(\mathbf{q}, \omega)$

$$\chi^{\pm 0}_{\boldsymbol{G}\boldsymbol{G}'}(\omega, \boldsymbol{q}) = \frac{2}{\Omega} \sum_{\boldsymbol{k}} \sum_{\nu,\nu'} \frac{\left(f_{\varepsilon_{\nu \boldsymbol{k}}} - f_{\varepsilon_{\nu' \, \mathbf{k}+\mathbf{q}}}\right) \rho^{\mathbf{kq}}_{\nu\nu'}(\boldsymbol{G}) \rho^{\mathbf{kq}}_{\nu\nu'}(\mathbf{G}')^*}{\omega + \varepsilon_{\nu \boldsymbol{k}} - \varepsilon_{\nu' \, \boldsymbol{k}+\boldsymbol{q}} \pm i\eta}$$

$$\rho^{\mathbf{kq}}_{\nu\nu'}(\boldsymbol{G}) = \sum_{\mathbf{G}'} \mathrm{C}^*_{\nu \mathbf{k}+\mathbf{G}'} \, \mathrm{C}_{\nu' \mathbf{k}+\mathbf{q}+\boldsymbol{G}+\mathbf{G}'}$$

Full Polarizability $\chi_{\boldsymbol{G}\boldsymbol{G}'} = \chi^0_{\boldsymbol{G}\boldsymbol{G}'} + (\chi^0 v \chi)_{\boldsymbol{G}\boldsymbol{G}'} = [\chi^0 (1 - v\chi_0)^{-1}]_{\boldsymbol{G}\boldsymbol{G}'}$

Screening (Plasmon Properties)

$$(\epsilon^{-1})_{\boldsymbol{G}\boldsymbol{G}'} = (1 + v\chi)_{\boldsymbol{G}\boldsymbol{G}'}$$

$$\approx [(1 - v\chi^0)^{-1}]_{\boldsymbol{G}\boldsymbol{G}'}$$

Dynamically screened interaction

$$W(\boldsymbol{r}, \boldsymbol{r}') = \int \frac{d^3 r''}{4\pi} \frac{\epsilon^{-1}(\boldsymbol{r}, \boldsymbol{r}'')}{|\boldsymbol{r}'' - \boldsymbol{r}'|}$$

Macroscopic Average

$$\epsilon_{\alpha\alpha}(q,\omega)^{-1} = [\epsilon_{\mathbf{GG'}}(q\boldsymbol{u}_{\alpha},\omega)^{-1}]_{\mathbf{G=G'=0}}$$

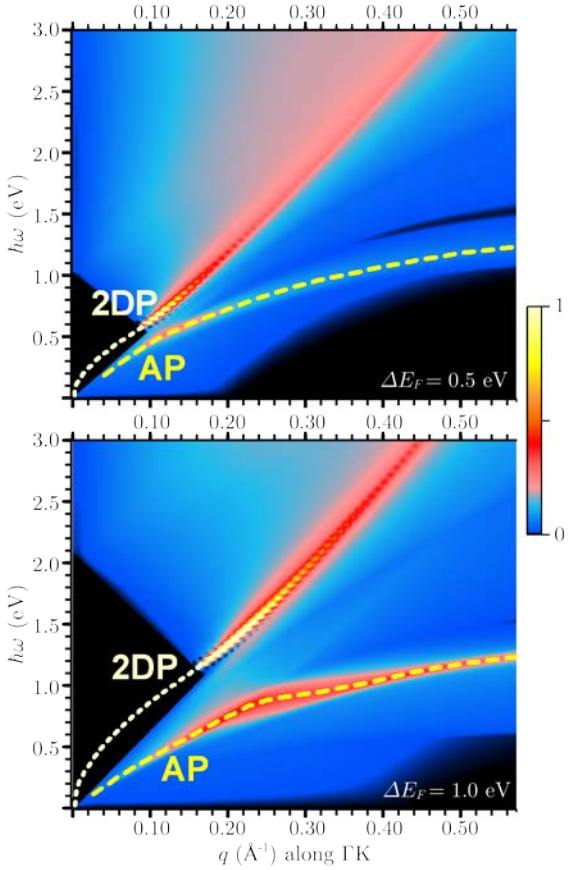
$\mathrm{Re}[\epsilon_{\alpha\alpha}(q,\nu)] = 0$ **Plasmon Resonances**

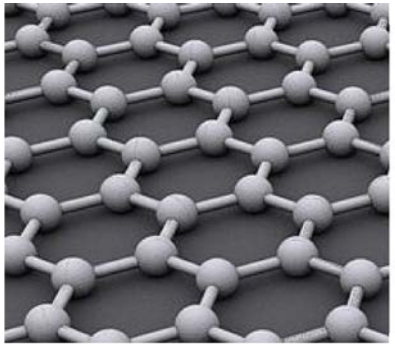
$\mathrm{Im}[\epsilon_{\alpha\alpha}(q,\nu)]$ **Absorption Spectrum**

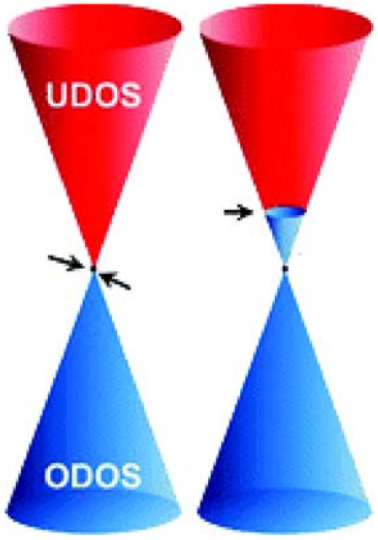
$-\mathrm{Im}[\epsilon_{\alpha\alpha}(q,\nu)^{-1}]$ **Loss Function (Plasmon Spectrum)**

M. Pisarra, A. Sindona, P. Riccardi, V. M. Silkin, J. M, Pitarke, **New Journal of Physics** 16, 083003 (2014); M. Pisarra, A. Sindona, M. Gravina, V. M. Silkin, J. M. Pitarke, **Physical Review B** 93, 035440 (2016); C. Vacacela Gomez, M. Pisarra, M. Gravina, J. M. Pitarke and A. Sindona, **Physical Review Letters** 117, 116801; (2016); C. Vacacela Gomez, M. Pisarra, M. Gravina and A. Sindona, **Physical Review B** 00, 005400 (2017)

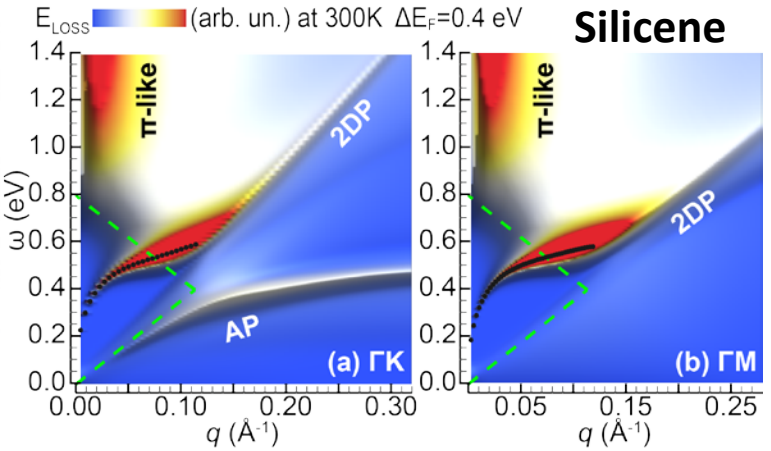
Graphene

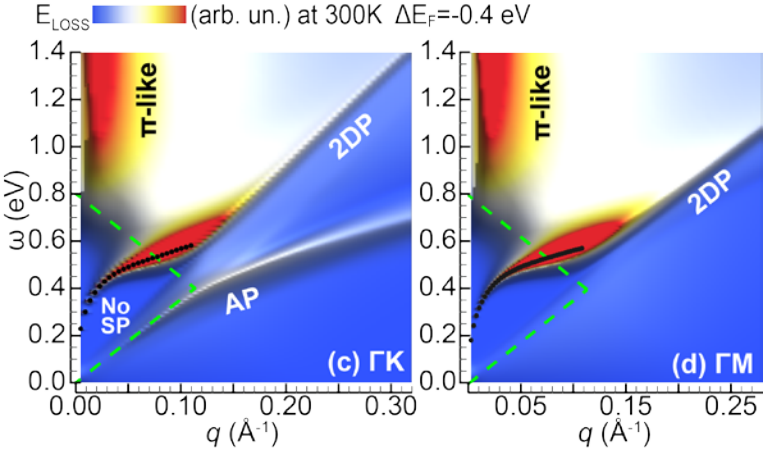


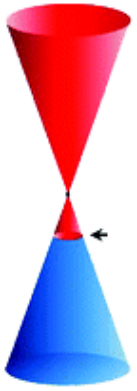




Silicene

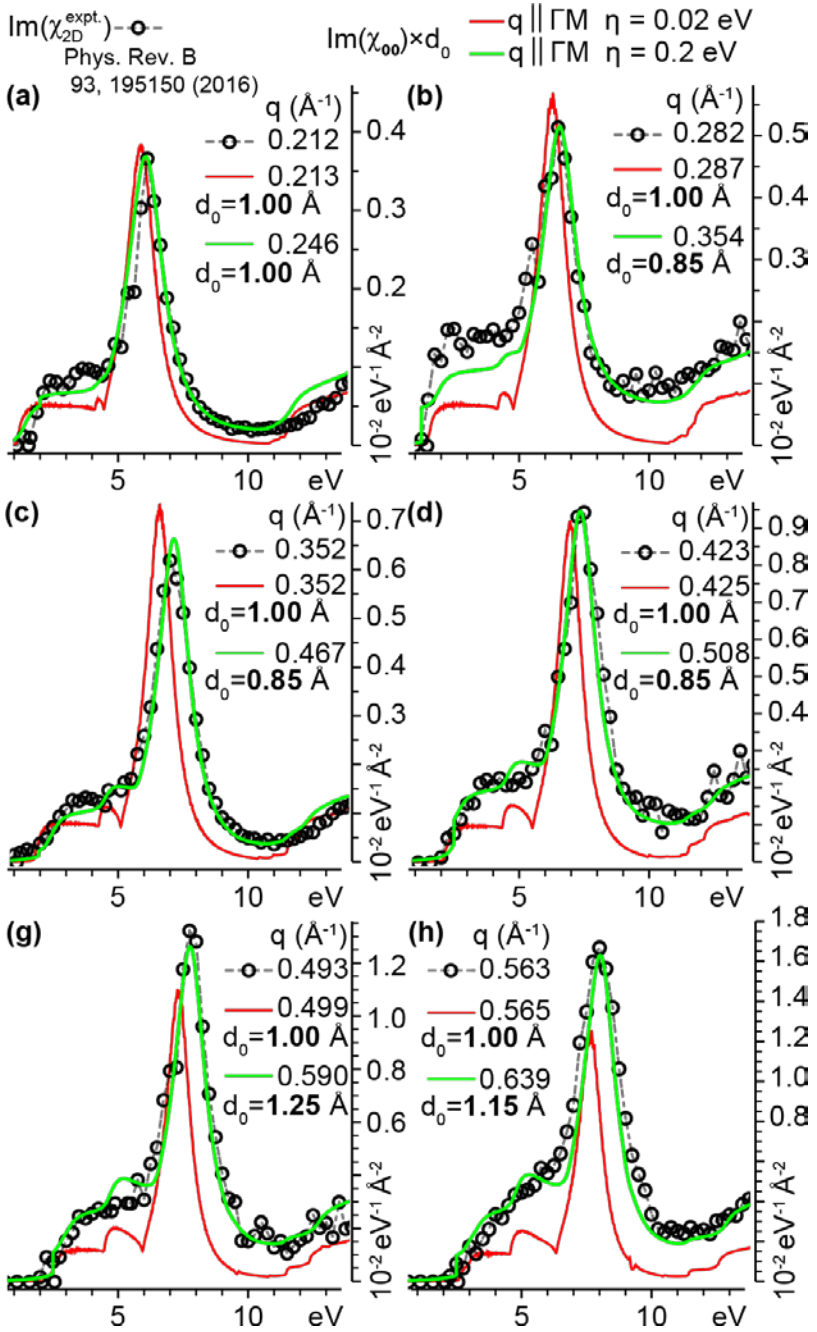






~1000 Core h per q point!!!

Ab initio calculation of α in graphene



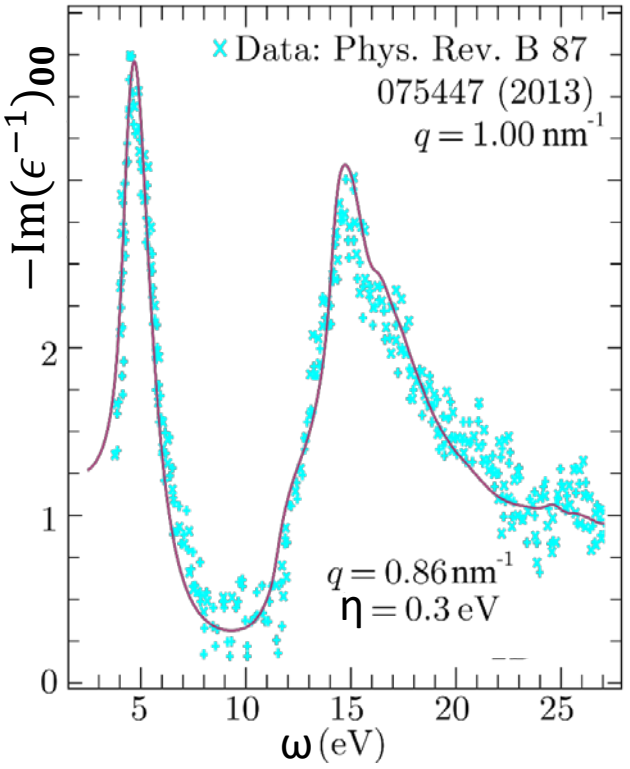
Dynamic Screening

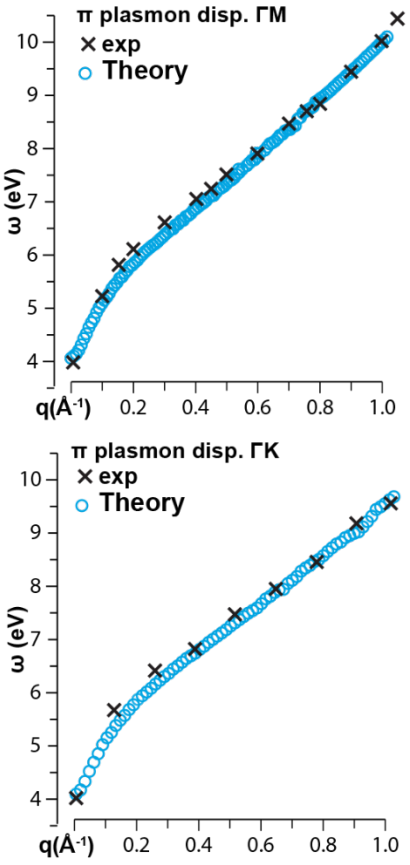
$$(\epsilon^{-1})_{GG'} = (1 + v\chi)_{GG'}$$

$$\chi_{GG'} = (\chi^0 + \chi^0 v\chi)_{GG'}$$
$$= [\chi^0(1 - v\chi^0)^{-1}]_{GG'}$$

Effective electron-electron interaction

$$v_{GG'} = \frac{2\pi}{|q+g|}\int_{-L/2}^{L/2} dz \int_{-L/2}^{L/2} dz' e^{iG_z z - iG'_z z' - |q+g||z-z'|}$$





Dynamic Screening

$$\chi^{+0}_{GG'} = \frac{2}{\Omega}\sum_{k}\sum_{\nu,\nu'}\frac{\left(f_{\varepsilon_{\nu k}} - f_{\varepsilon_{\nu' \, k+q}}\right)\rho^{kq}_{\nu\nu'}(G)\rho^{kq}_{\nu\nu'}(G')^{*}}{\omega + \varepsilon_{\nu k} - \varepsilon_{\nu' \, k+q} + i\eta}$$

$$\chi_{GG'} = [\chi^{0}(1 - v\chi^{0})^{-1}]_{GG'}$$

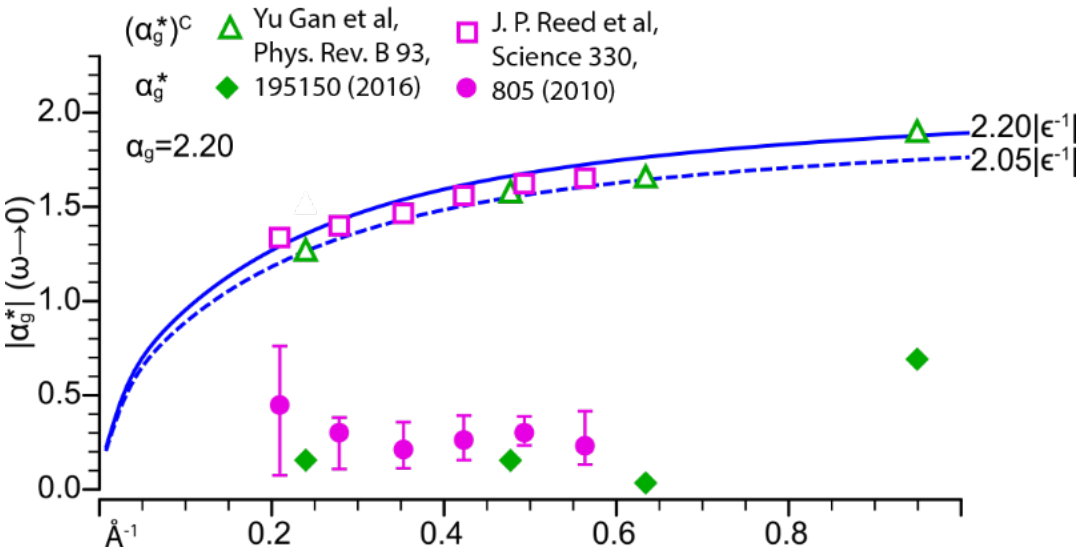
Effective electron-electron interaction

$$v_{GG'} = \frac{2\pi}{|q+g|}\int_{-L/2}^{L/2} dz \int_{-L/2}^{L/2} dz' e^{iG_z z - iG'_z z' - |q+g||z-z'|}$$

Reconstruction of the dressed fine-structure constant

$$\alpha_g^*(\mathbf{q},\omega) = \alpha_g\left[1 + V_{2D}(\mathbf{q})\chi_{2D}(\mathbf{q},\omega)\right]$$

$$(\alpha_g^*)^c(\mathbf{q},\omega) = \alpha_g\left[1 + \langle v_{00}(\mathbf{q})\rangle\chi_{2D}(\mathbf{q},\omega)\right]$$



Ab initio calculation of α in graphene

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HPC Resources

Requirements:
Large cells (>50 atoms) or **supercells** (4x4 or more!)
Large k-space grids (up to 2400x2400!) to properly sample the Dirac cones features
Multiple-Step simulations: DFT-SCR-GW-BSE & post-processing (DOS,PDOS ect)

Average Core h per simulations on a case study:
-5000 Core h for a typical relaxation run + scf + nscf
(x # systems) = 100.000 Core h for all DFT runs
-6000 Core h for a typical GW run
(x # systems x convergence tests) = 300.000 Core h for GW runs
-4000 Core h for a typical BSE run
(x # systems x convergence tests) = 200.000 Core h for BSE runs

Suggested Reading

1. A. Sindona, M. Pisarra, C. Vacacela Gomez, P. Riccardi, G. Falcone, and S. Bellucci, “Calibration of the fine-structure constant of graphene by time-dependent density-functional theory”, **Physical Review B** 96, 201408(R) – Published 17 November 2017
2. A. Sindona, A. Cupolillo, et al., “Interband π-like plasmon in silicene grown on silver”, arXiv:1708.03858 [cond-mat.mtrl-sci], to appear as a rapid communication in **Physical Review B** (21 dec 2017)
3. C. Vacacela Gomez, M. Pisarra, M. Gravina, J. M. Pitarke and A. Sindona, "Plasmon Modes of Graphene Nanoribbons with Periodic Planar Arrangements", **Physical Review Letters** 117, 116801 (2016)
4. A. Sindona et al, “Orthogonality Catastrophe and Decoherence in a Trapped-Fermion Environment”, **Physical Review Letters** 111, 165303 (2013)

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