Is quantum theory exact? The endeavor for the theory beyond standard quantum mechanics. Second Edition FQT2015

Electromagnetic characterization of graphene and graphene nanoribbons via ab-initio permittivity simulations

S. Bellucci TH activities coordinator (1999-2003 & 2011-2015)

NEXT Nanotechnology Laboratory
INFN-Laboratori Nazionali Frascati

Frascati, Sep 23, 2015

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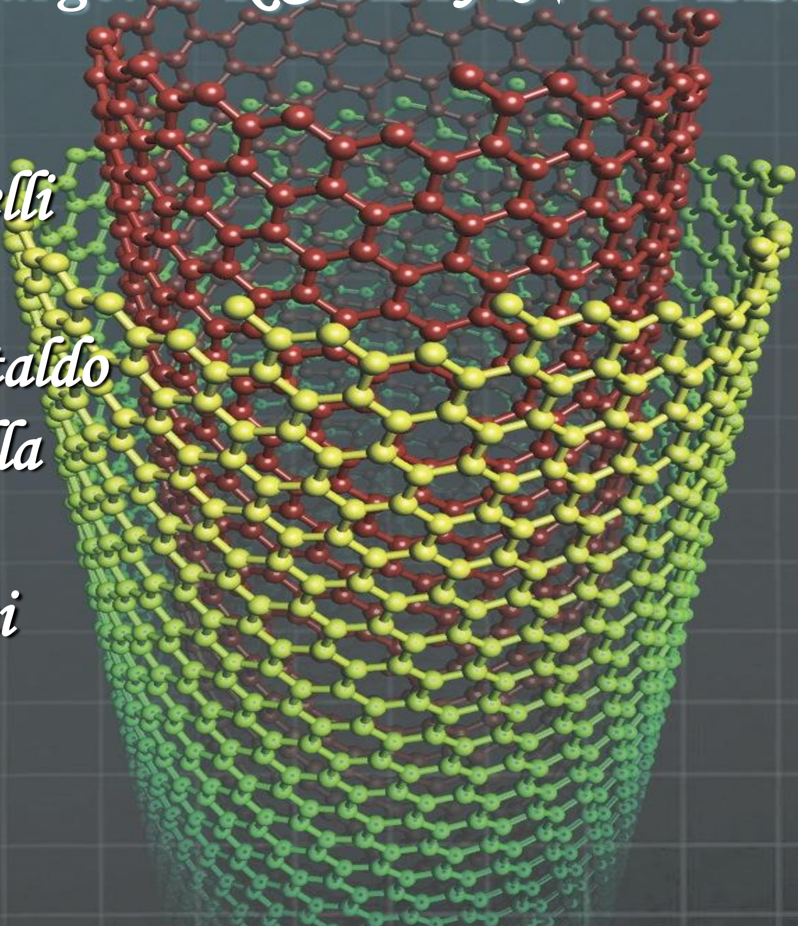
Nano Technology Laboratories

NanosciencE eXperiments for Technology

Lab in charge: *DR STEFANO BELLUCCI*



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Il MONDO
della SCUOLA,
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insieme per
l'INNOVAZIONE:

NANOSCIENZA E
NANOTECNOLOGIA

I.T.I.S. "G.Galilei" di Arezzo, 11 e 12 marzo 2013

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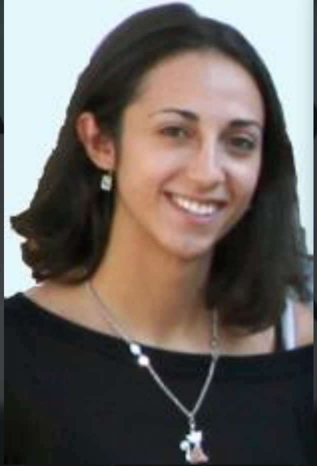
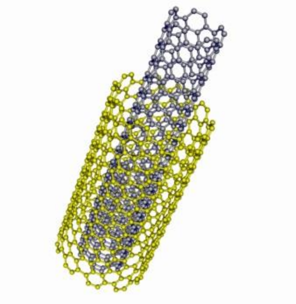


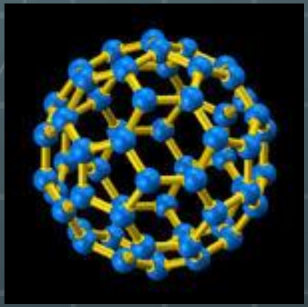
Nanotechnology

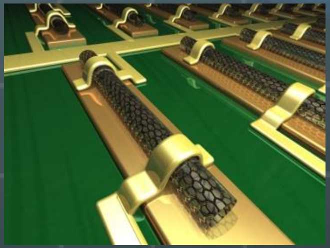
Nanotechnology is the postulated ability to manufacture objects and structures with atomic precision, literally atom by atom.

This would mirror the abilities of living cells, which do exactly the same thing, although based on evolution and not design.

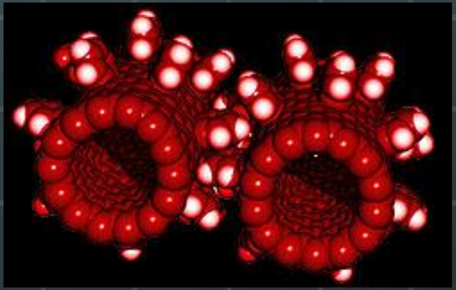
Simple applications involve the creation of new and powerful materials, perfect diamond in bulk quantities and a tool to manipulate objects on any scale.







More *advanced* applications would involve massively parallel nanocomputers, self-replication and more or less smart nanodevices able to interact with their surroundings.



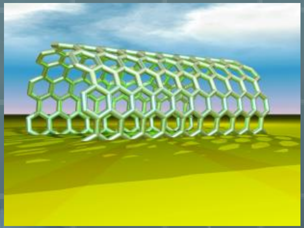
e-mail: bellucci@lnf.infn.it

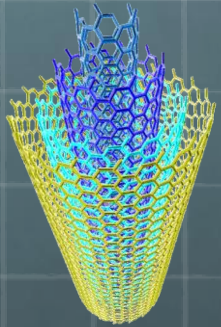
Carbon Nanotubes

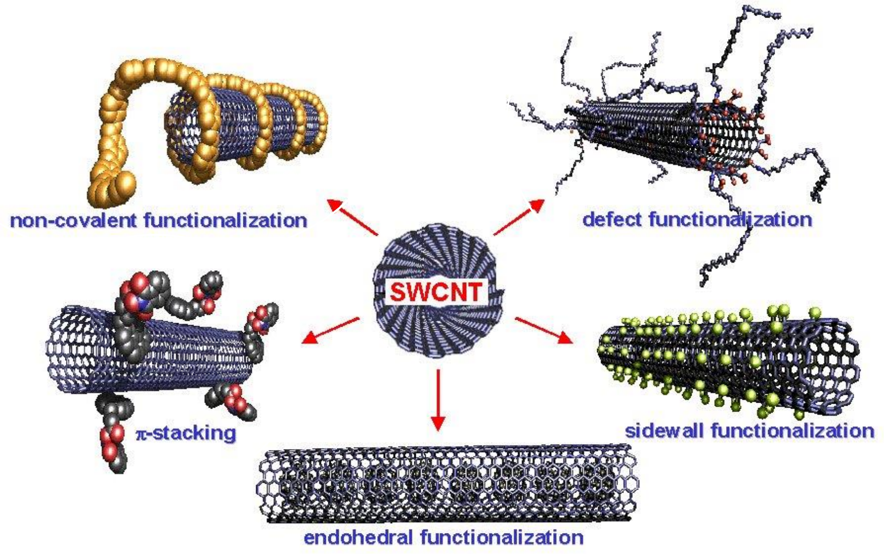
Carbon nanotubes, long and thin cylinders of carbon, discovered 24 years ago, though existing for a long time.

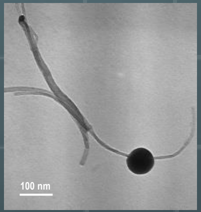
They can be thought of a sheet of graphite (a hexagonal lattice of carbon) rolled up into a cylinder.

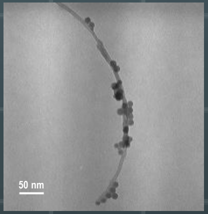
Carbon nanotubes are characterized by unique structural, mechanical, electrical and chemical properties and they have been widely studied and used in the realization of composite nanomaterials.

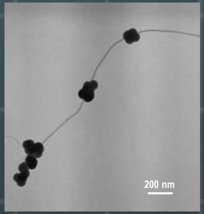


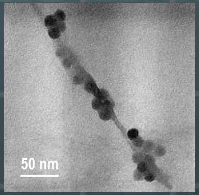


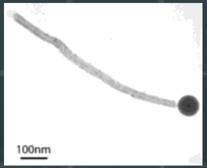


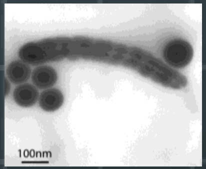












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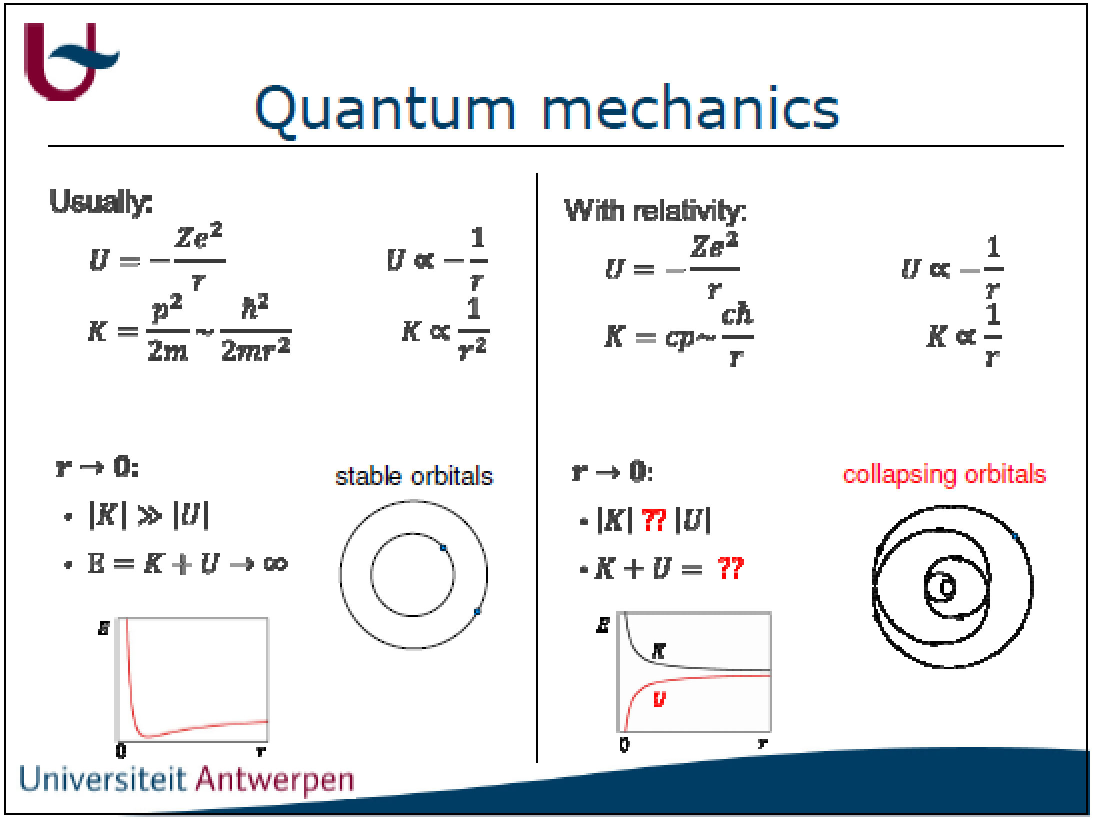


Quantum mechanics

Usually:

$U = -\frac{Ze^2}{r}$ $\qquad U \propto -\frac{1}{r}$

$K = \frac{p^2}{2m} \sim \frac{\hbar^2}{2mr^2}$ $\qquad K \propto \frac{1}{r^2}$

$r \to 0$:

- $|K| \gg |U|$
- $E = K + U \to \infty$

stable orbitals

With relativity:

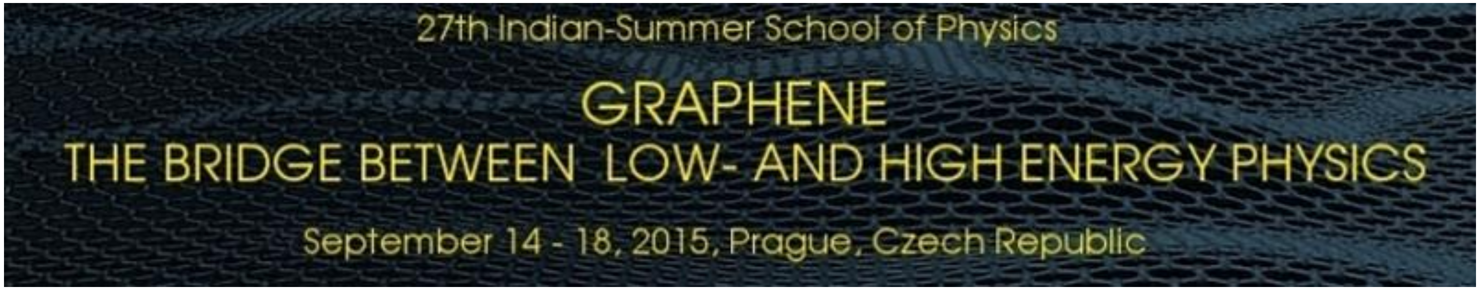
$U = -\frac{Ze^2}{r}$ $\qquad U \propto -\frac{1}{r}$

$K = cp \sim \frac{c\hbar}{r}$ $\qquad K \propto \frac{1}{r}$

$r \to 0$:

- $|K|$?? $|U|$
- $K + U =$??

collapsing orbitals



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THE BRIDGE BETWEEN LOW- AND HIGH ENERGY PHYSICS

September 14 - 18, 2015, Prague, Czech Republic

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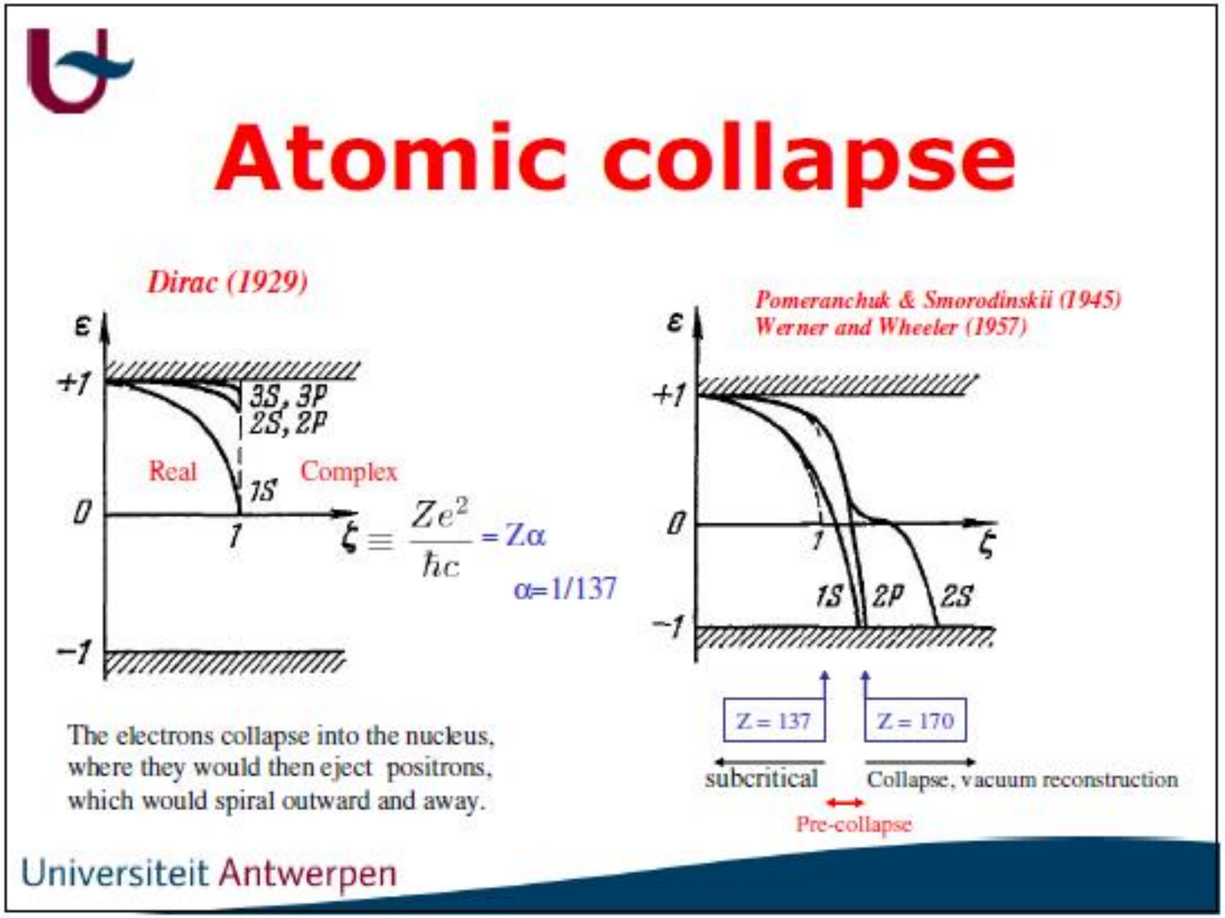

Atomic collapse

Dirac (1929)

$$\zeta \equiv \frac{Ze^2}{\hbar c} = Z\alpha$$

α=1/137

The electrons collapse into the nucleus, where they would then eject positrons, which would spiral outward and away.

Pomeranchuk & Smorodinskii (1945)
Werner and Wheeler (1957)

Z = 137

Z = 170

subcritical

Collapse, vacuum reconstruction

Pre-collapse

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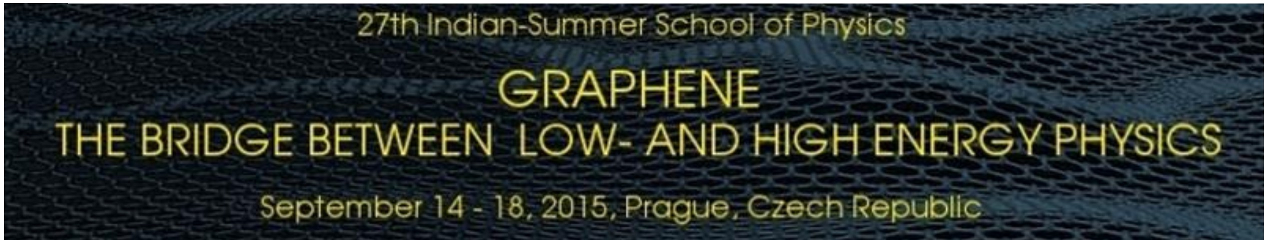

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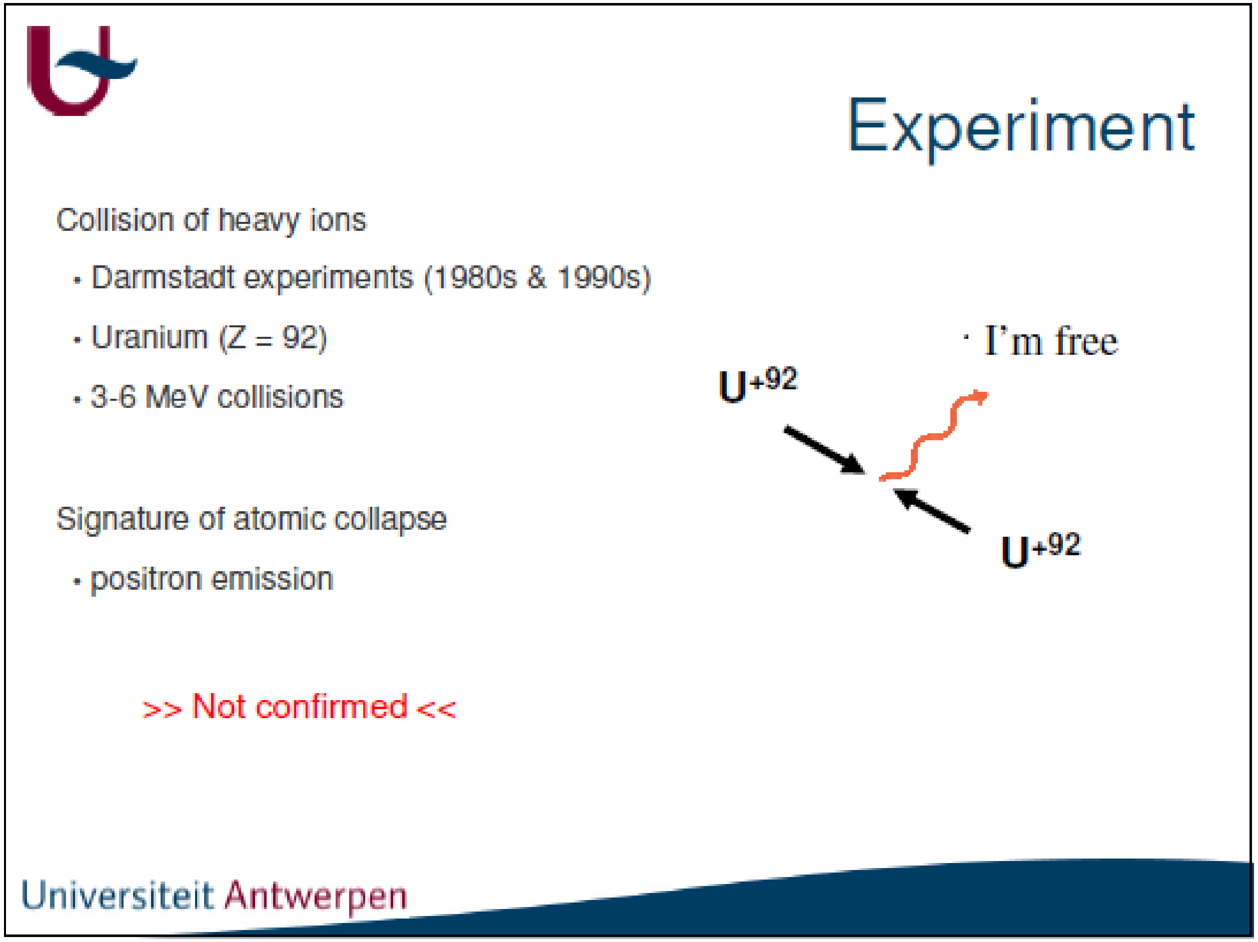

Experiment

Collision of heavy ions

- Darmstadt experiments (1980s & 1990s)
- Uranium (Z = 92)
- 3-6 MeV collisions

Signature of atomic collapse

- positron emission

>> Not confirmed <<

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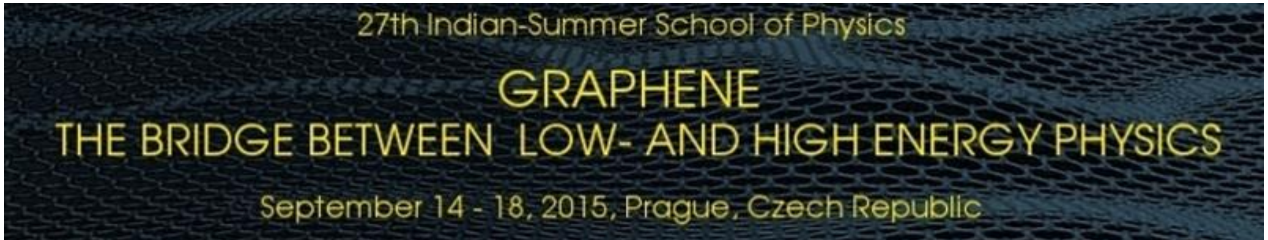

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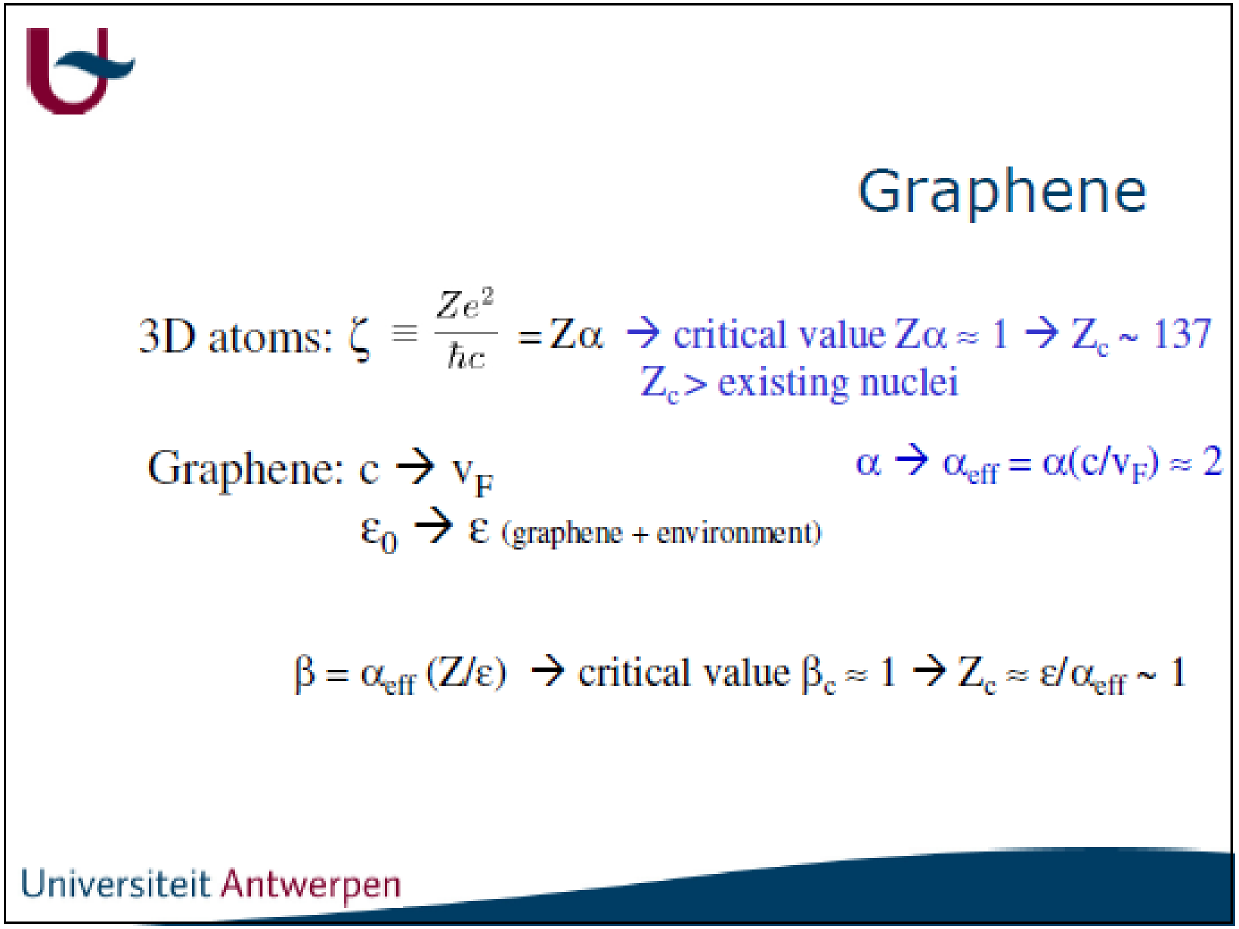

Graphene

3D atoms: $\zeta \equiv \frac{Ze^2}{\hbar c} = Z\alpha$ → critical value $Z\alpha \approx 1$ → $Z_c \sim 137$

$Z_c >$ existing nuclei

Graphene: $c \rightarrow v_F$

$\alpha \rightarrow \alpha_{eff} = \alpha(c/v_F) \approx 2$

$\varepsilon_0 \rightarrow \varepsilon$ (graphene + environment)

$\beta = \alpha_{eff}\,(Z/\varepsilon)$ → critical value $\beta_c \approx 1$ → $Z_c \approx \varepsilon/\alpha_{eff} \sim 1$

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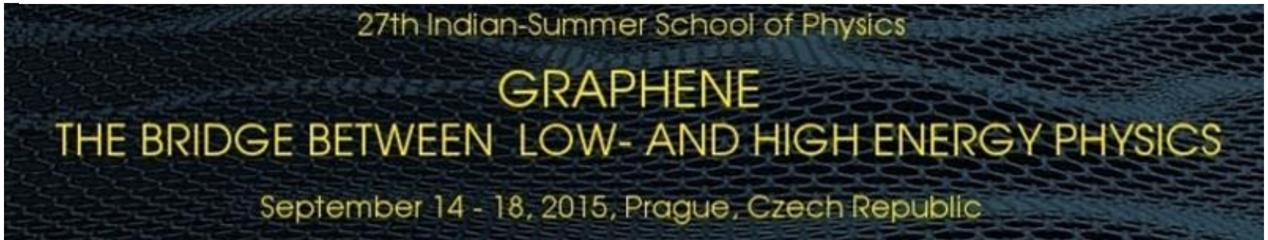

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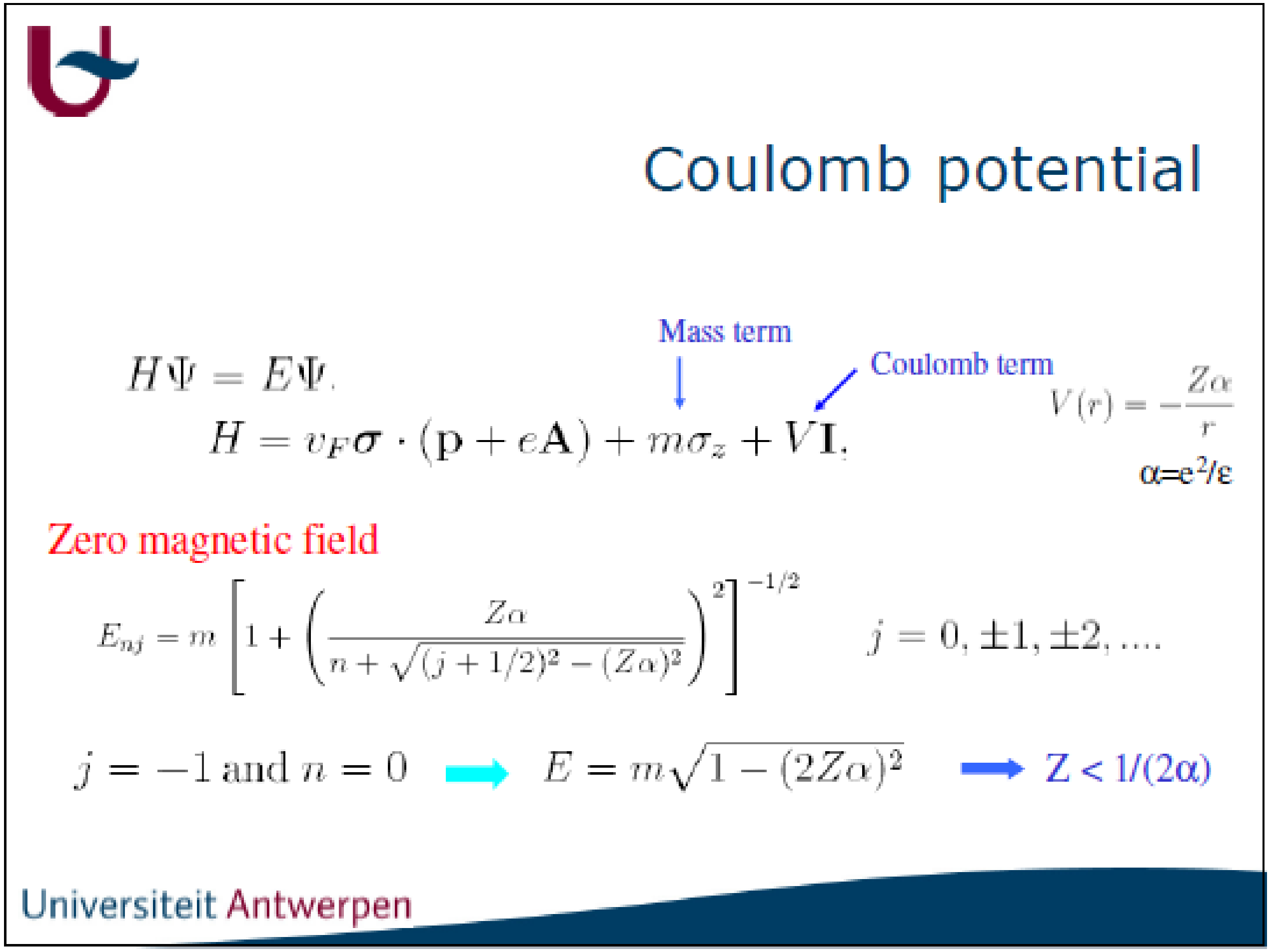

Coulomb potential

Mass term

Coulomb term

$$H\Psi = E\Psi.$$

$$H = v_F \boldsymbol{\sigma}\cdot(\mathrm{p}+e\mathbf{A}) + m\sigma_z + V\mathbf{I},$$

$$V(r) = -\frac{Z\alpha}{r}$$

$\alpha=e^2/\varepsilon$

Zero magnetic field

$$E_{nj} = m\left[1+\left(\frac{Z\alpha}{n+\sqrt{(j+1/2)^2-(Z\alpha)^2}}\right)^2\right]^{-1/2} \qquad j=0,\pm1,\pm2,\ldots.$$

$j=-1$ and $n=0$ ➡ $E=m\sqrt{1-(2Z\alpha)^2}$ ➡ $Z<1/(2\alpha)$

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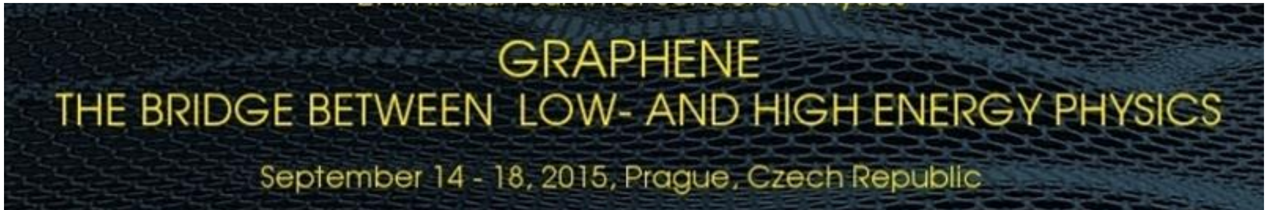

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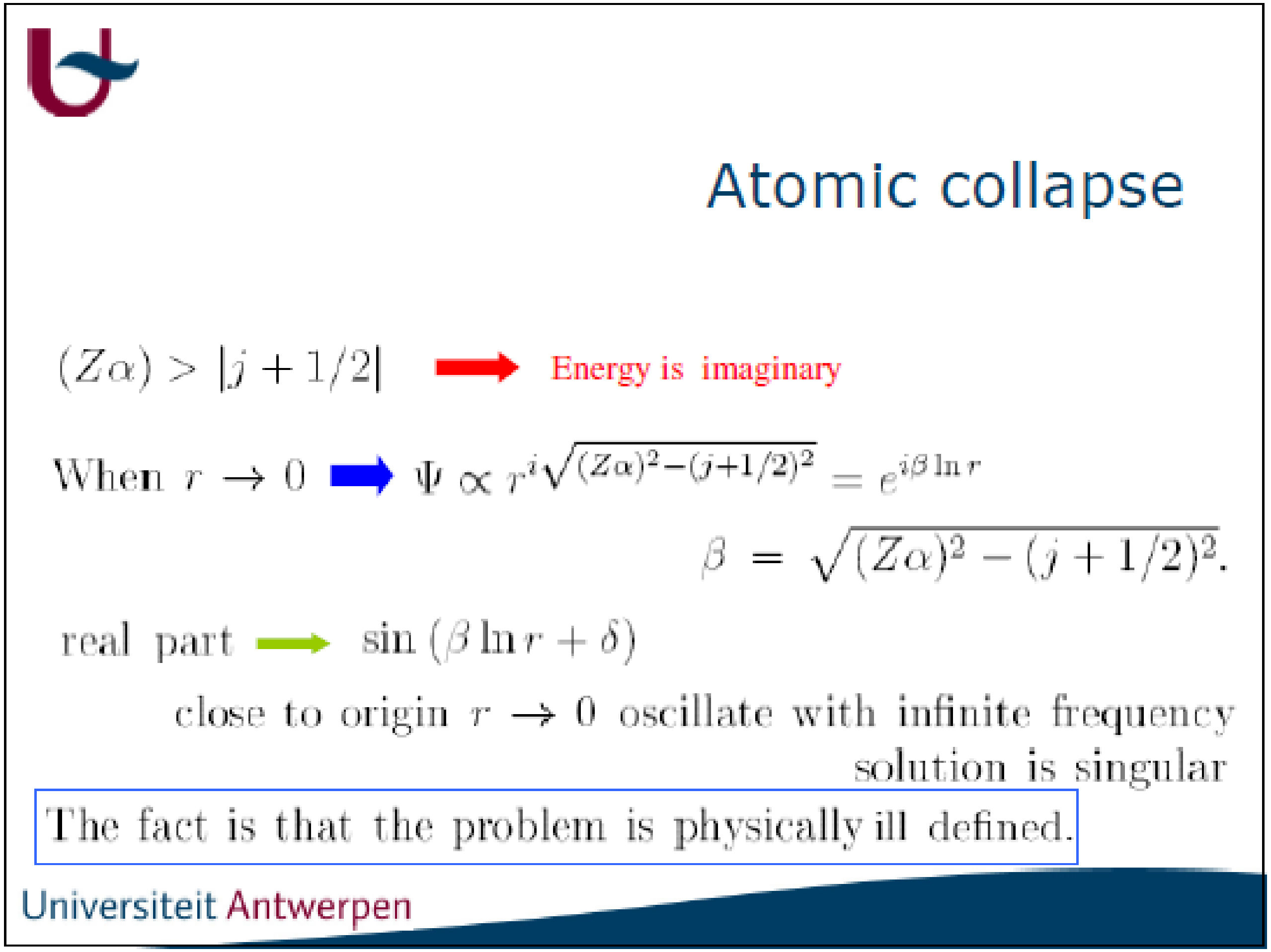

Atomic collapse

$(Z\alpha) > |j+1/2|$ ➡ Energy is imaginary

When $r \to 0$ ➡ $\Psi \propto r^{i\sqrt{(Z\alpha)^2-(j+1/2)^2}} = e^{i\beta \ln r}$

$$\beta = \sqrt{(Z\alpha)^2 - (j+1/2)^2}.$$

real part ➡ $\sin(\beta \ln r + \delta)$

close to origin $r \to 0$ oscillate with infinite frequency

solution is singular

The fact is that the problem is physically ill defined.

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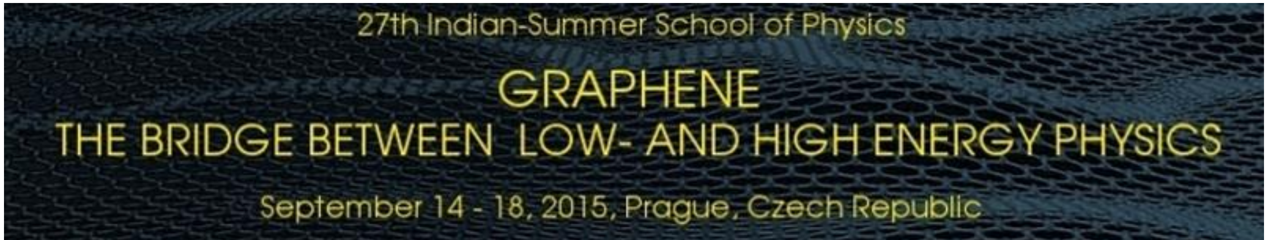

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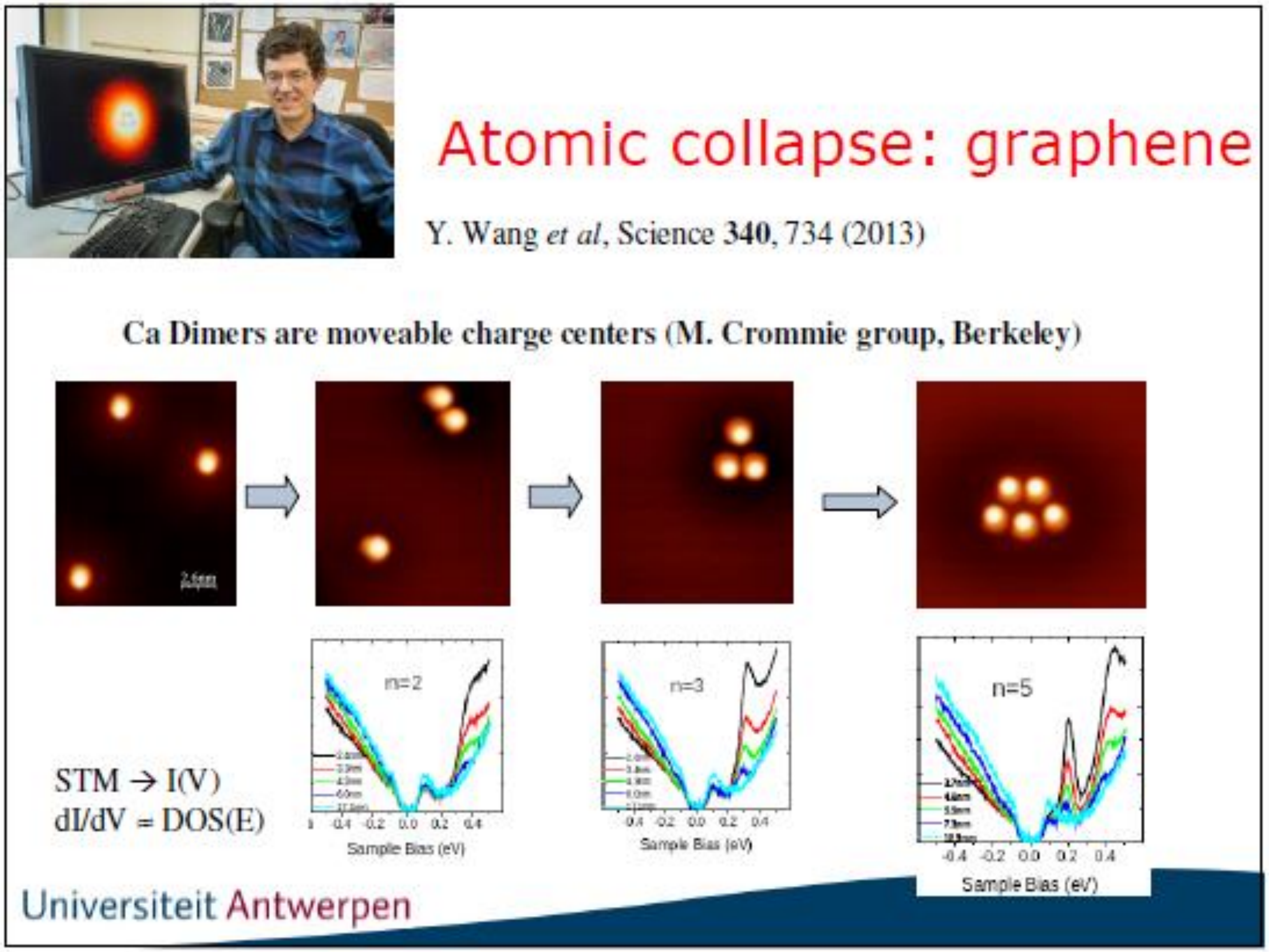

Atomic collapse: graphene

Y. Wang *et al*, Science **340**, 734 (2013)

Ca Dimers are moveable charge centers (M. Crommie group, Berkeley)

STM → I(V)

dI/dV = DOS(E)

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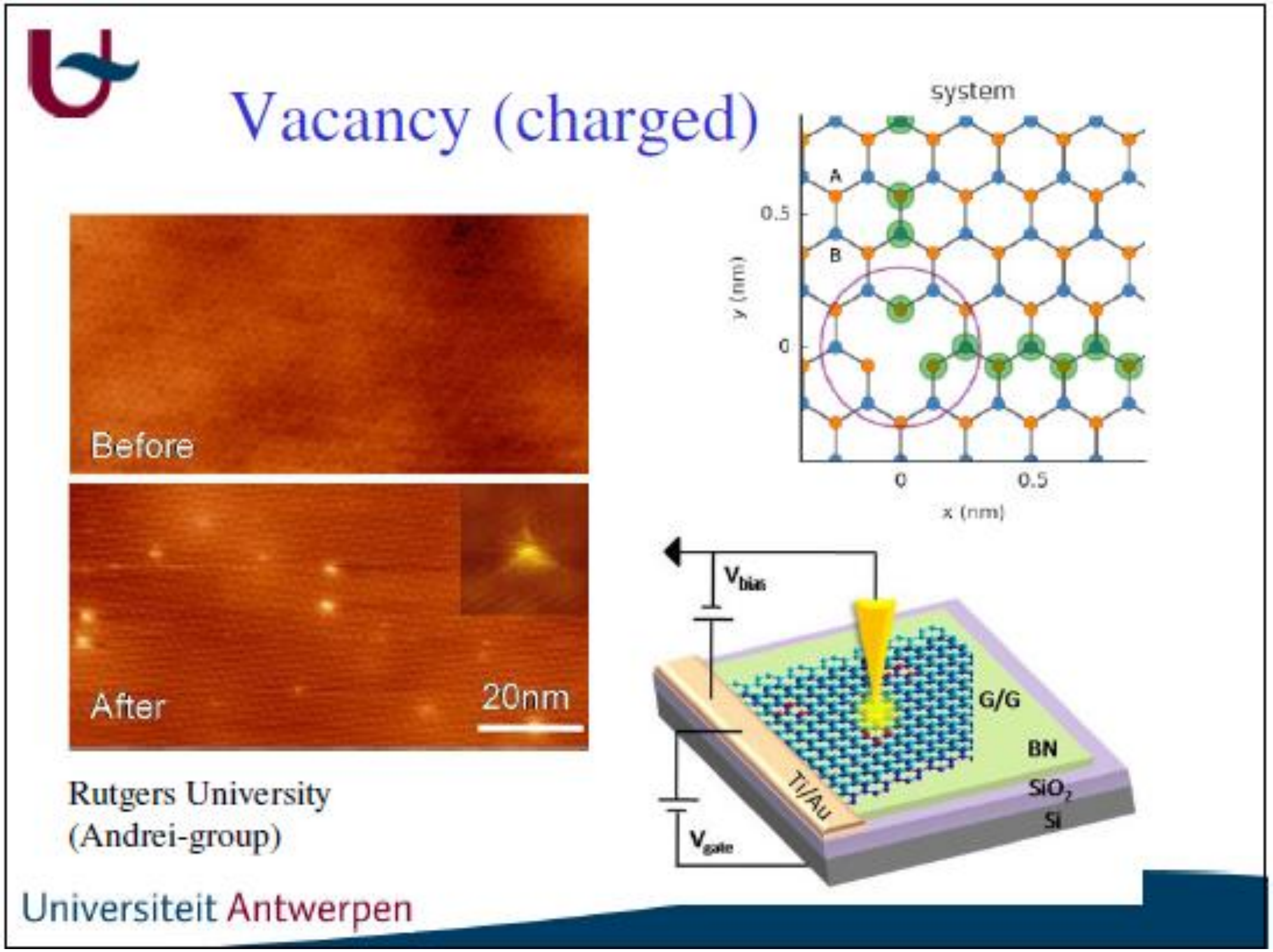

Vacancy (charged)

Before

After

20nm

Rutgers University
(Andrei-group)

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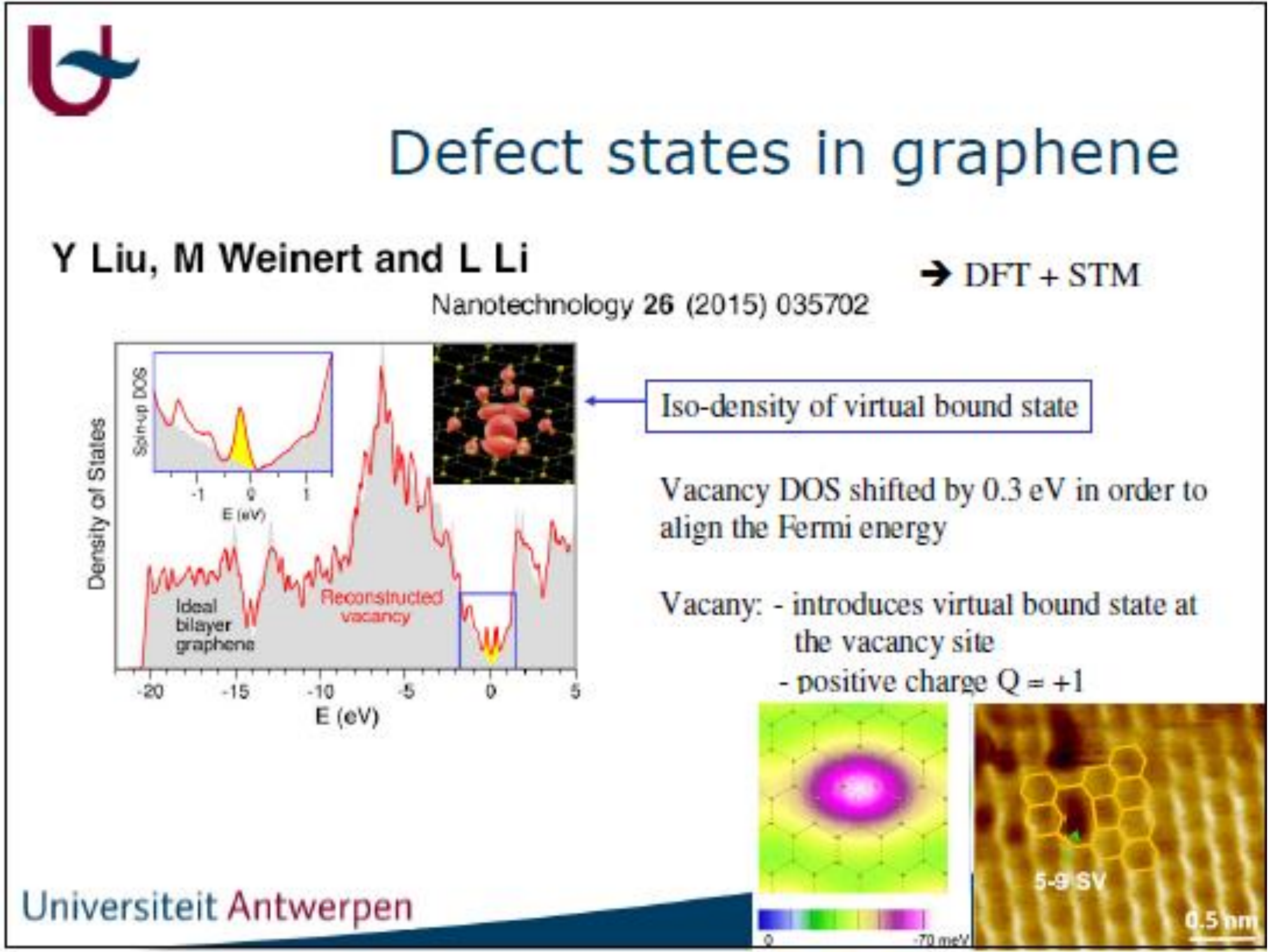

Defect states in graphene

Y Liu, M Weinert and L Li

Nanotechnology **26** (2015) 035702

→ DFT + STM

Iso-density of virtual bound state

Vacancy DOS shifted by 0.3 eV in order to align the Fermi energy

Vacany: - introduces virtual bound state at the vacancy site

- positive charge Q = +1

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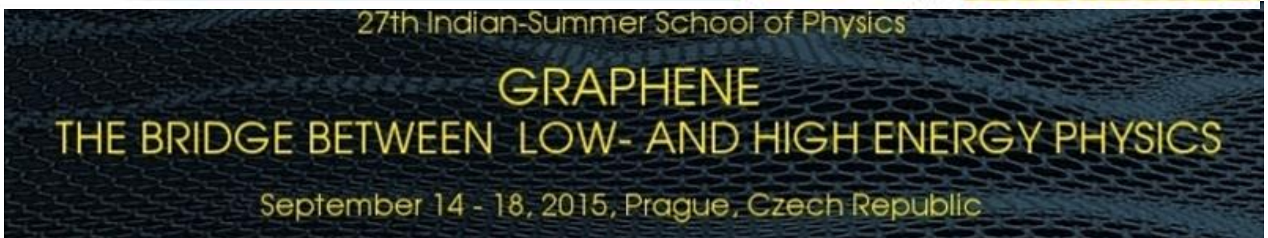

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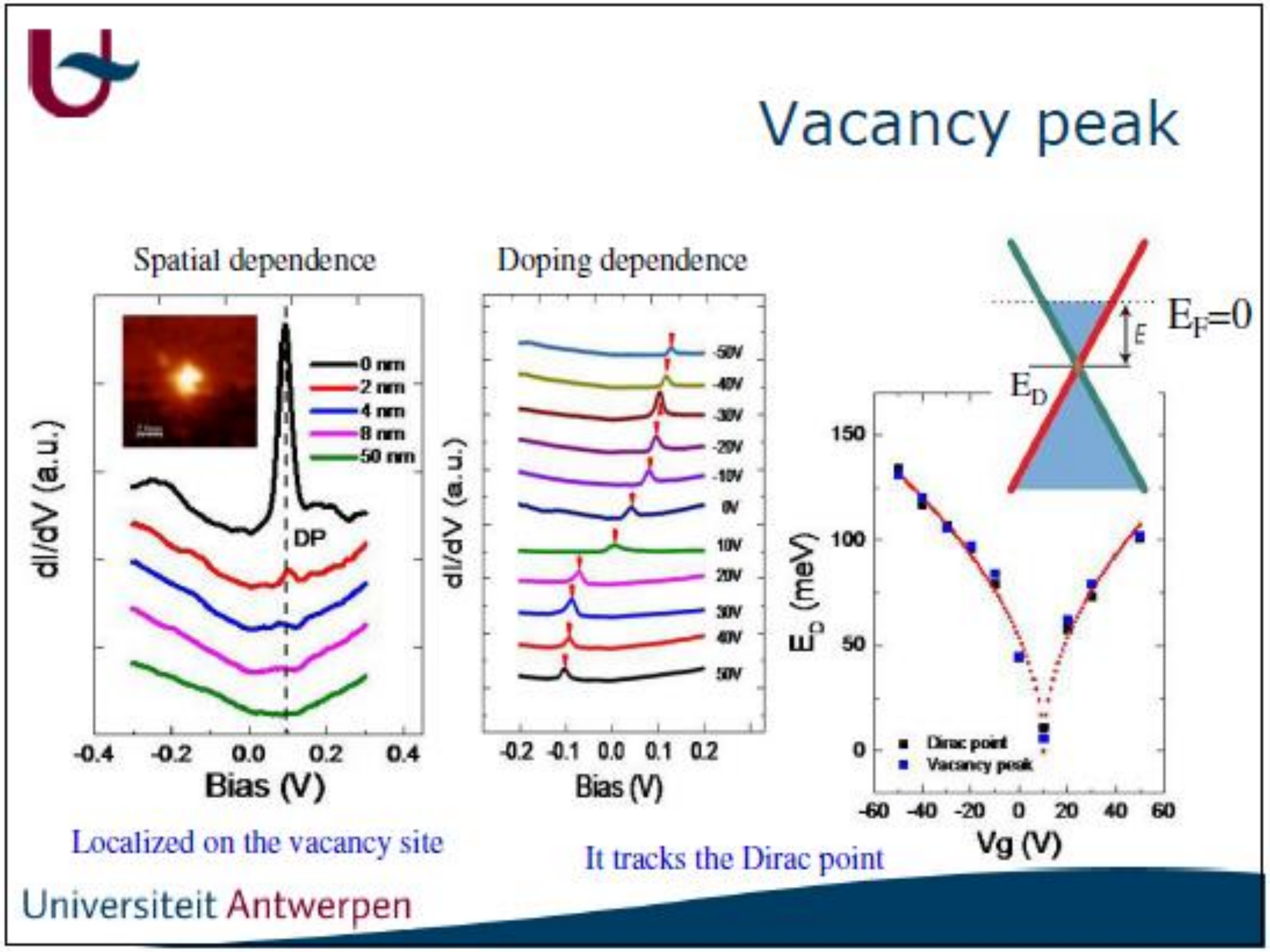

Vacancy peak

Localized on the vacancy site

It tracks the Dirac point

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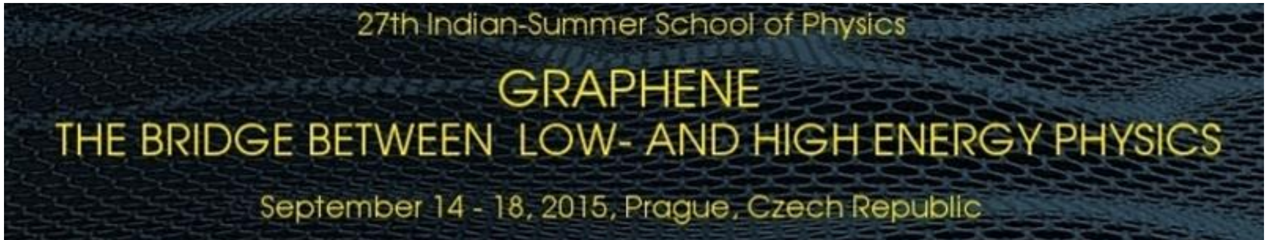

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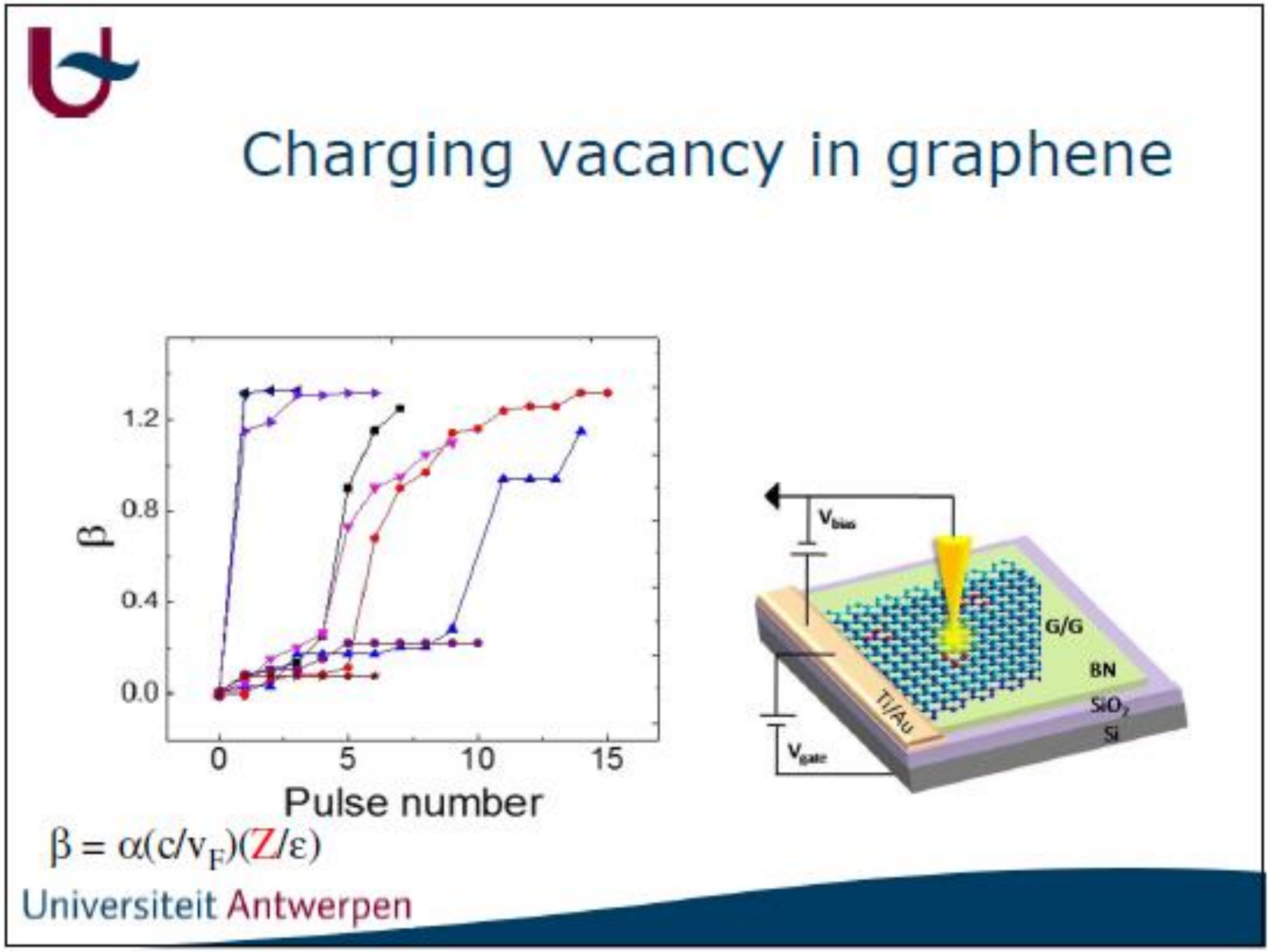

Charging vacancy in graphene

$\beta = \alpha(c/v_F)(Z/\varepsilon)$

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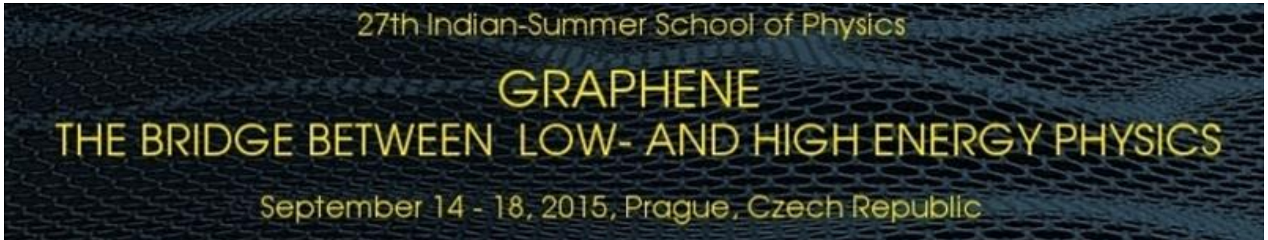

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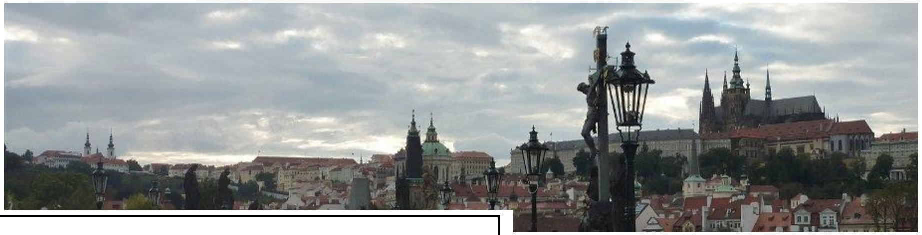
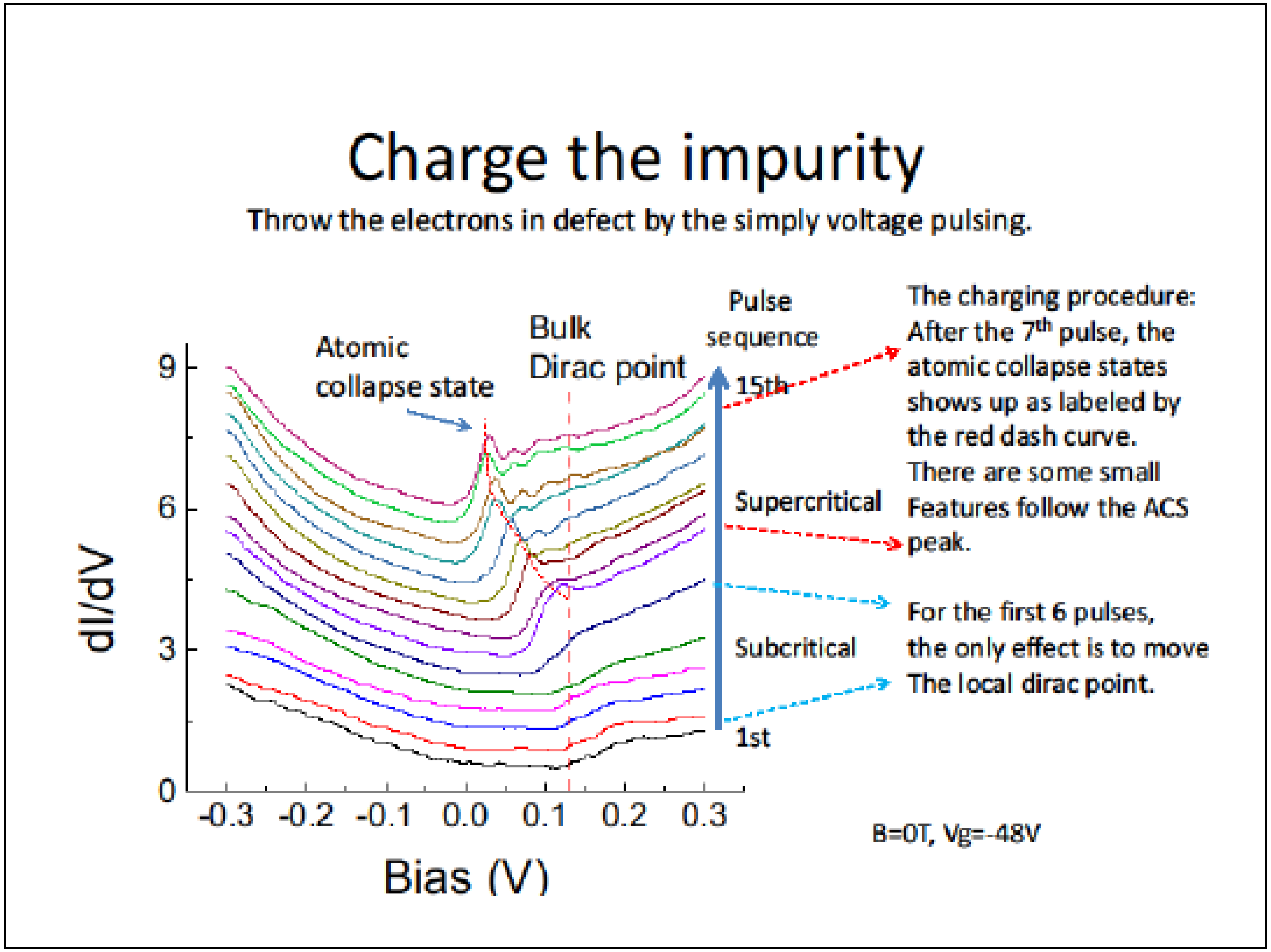




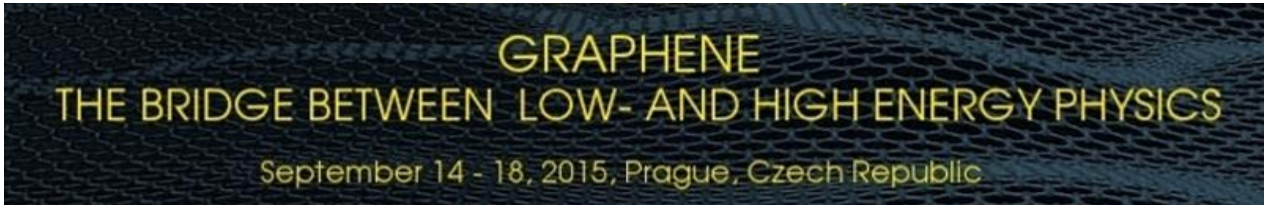
Charge the impurity

Throw the electrons in defect by the simply voltage pulsing.

The charging procedure:
After the 7th pulse, the
atomic collapse states
shows up as labeled by
the red dash curve.
There are some small
Features follow the ACS
peak.

For the first 6 pulses,
the only effect is to move
The local dirac point.

B=0T, Vg=-48V



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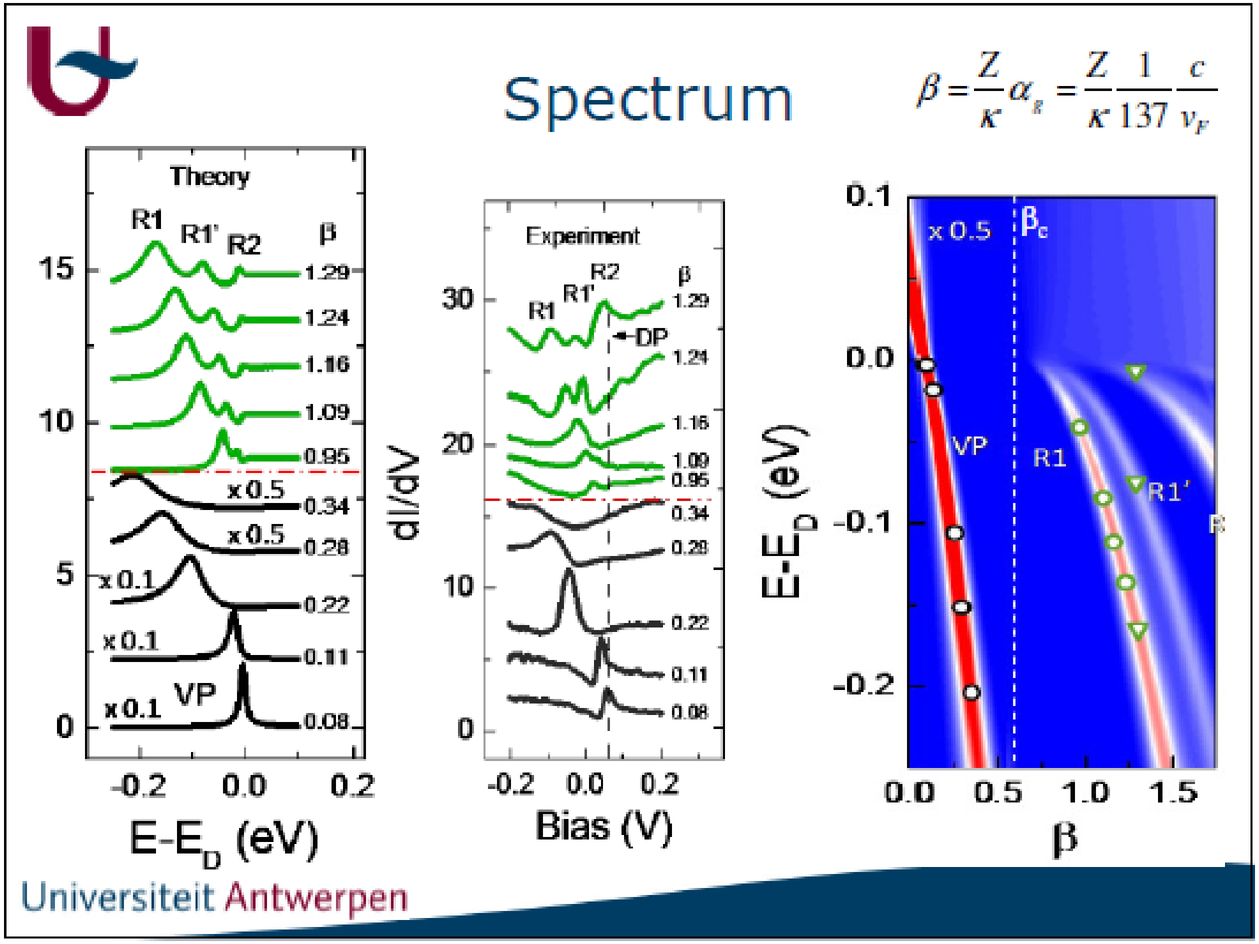

Spectrum

$$\beta=\frac{Z}{\kappa}\alpha_g=\frac{Z}{\kappa}\frac{1}{137}\frac{c}{v_F}$$

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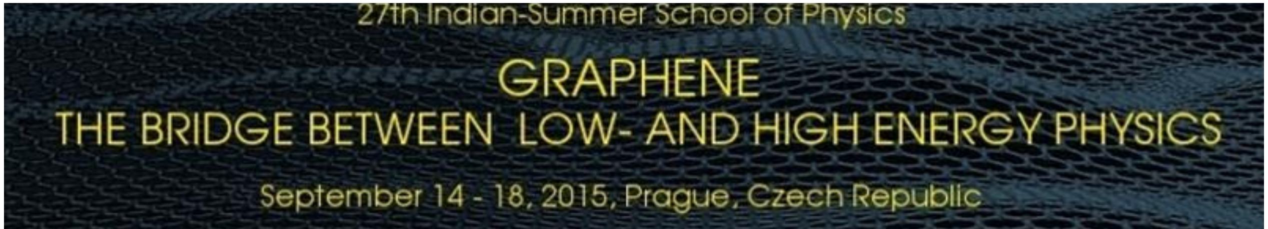

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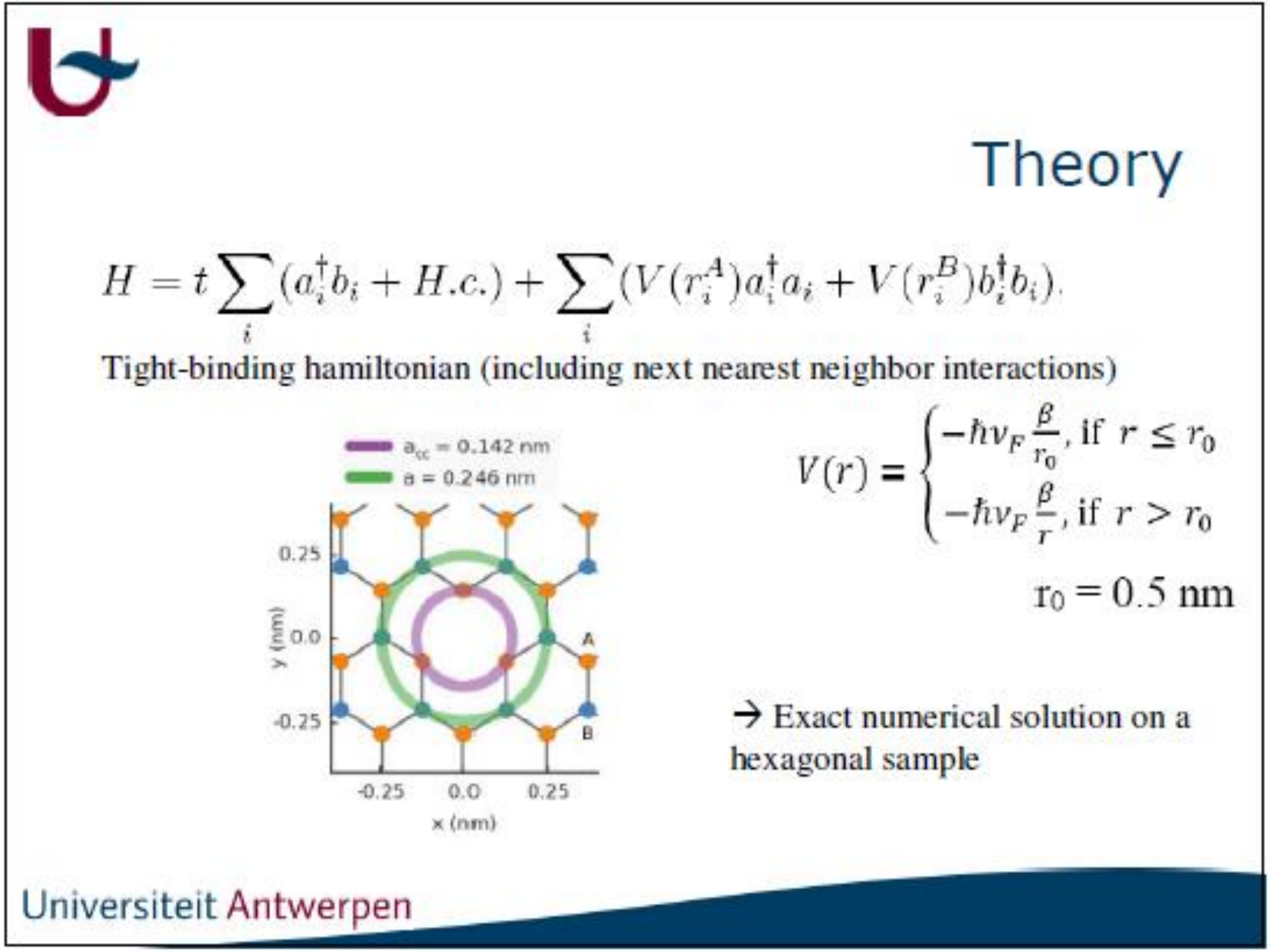

Theory

$$H = t\sum_i (a_i^\dagger b_i + H.c.) + \sum_i (V(r_i^A) a_i^\dagger a_i + V(r_i^B) b_i^\dagger b_i).$$

Tight-binding hamiltonian (including next nearest neighbor interactions)

$$V(r) = \begin{cases} -\hbar v_F \frac{\beta}{r_0}, \text{if } r \leq r_0 \\ -\hbar v_F \frac{\beta}{r}, \text{if } r > r_0 \end{cases}$$

$r_0 = 0.5$ nm

→ Exact numerical solution on a hexagonal sample

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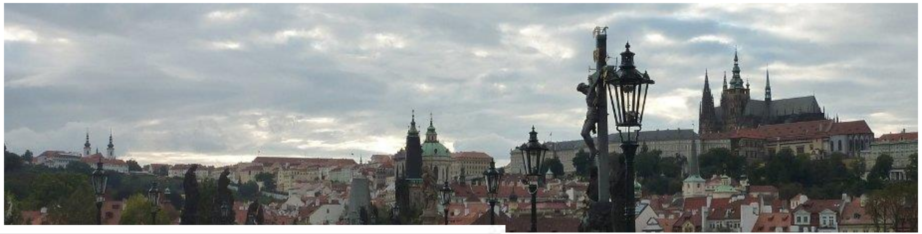

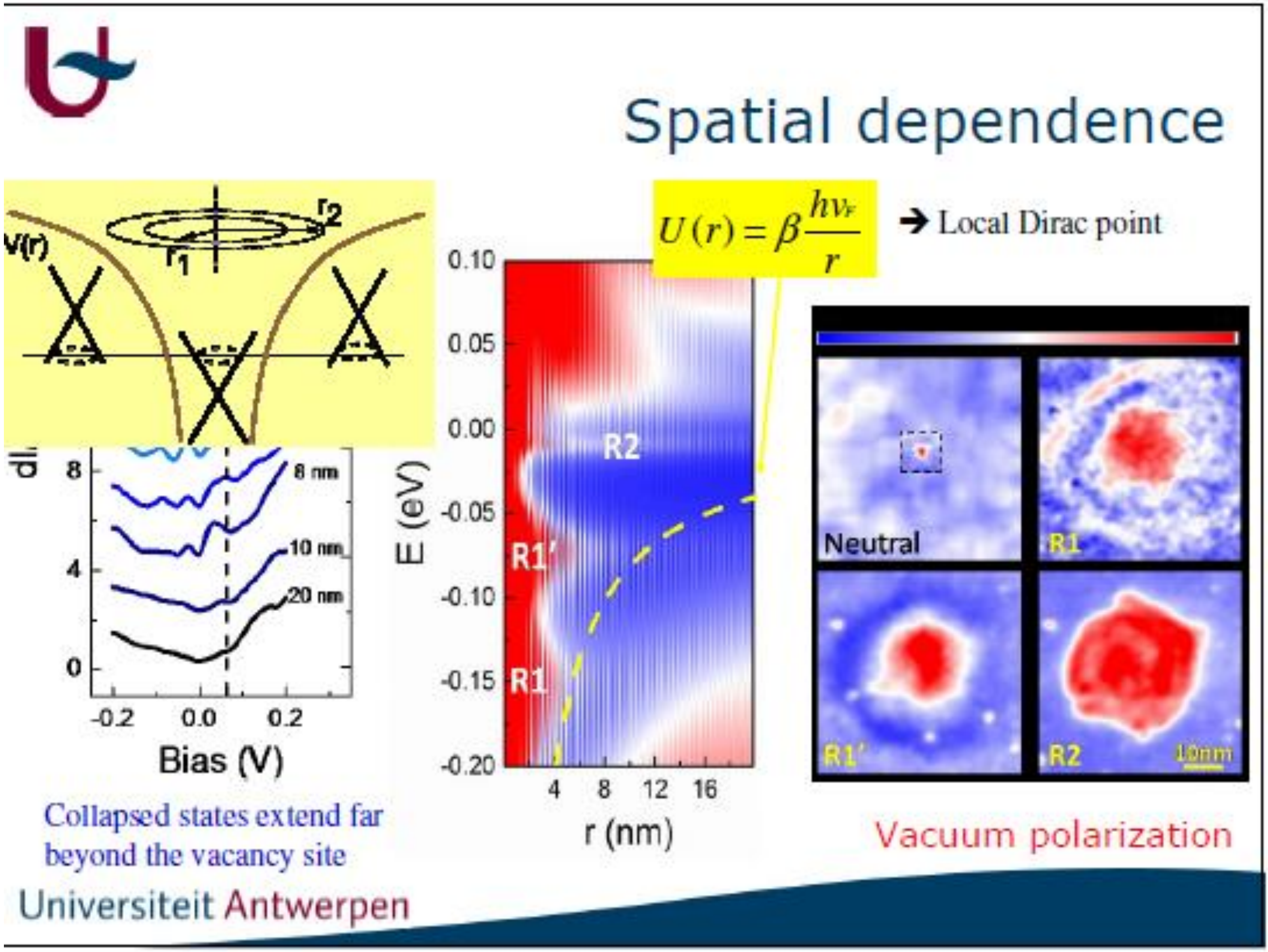

Spatial dependence

$U(r) = \beta \frac{h v_F}{r}$ → Local Dirac point

Collapsed states extend far beyond the vacancy site

Vacuum polarization

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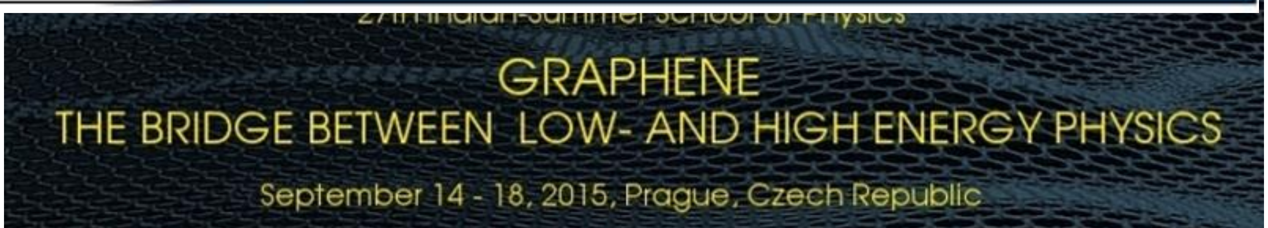

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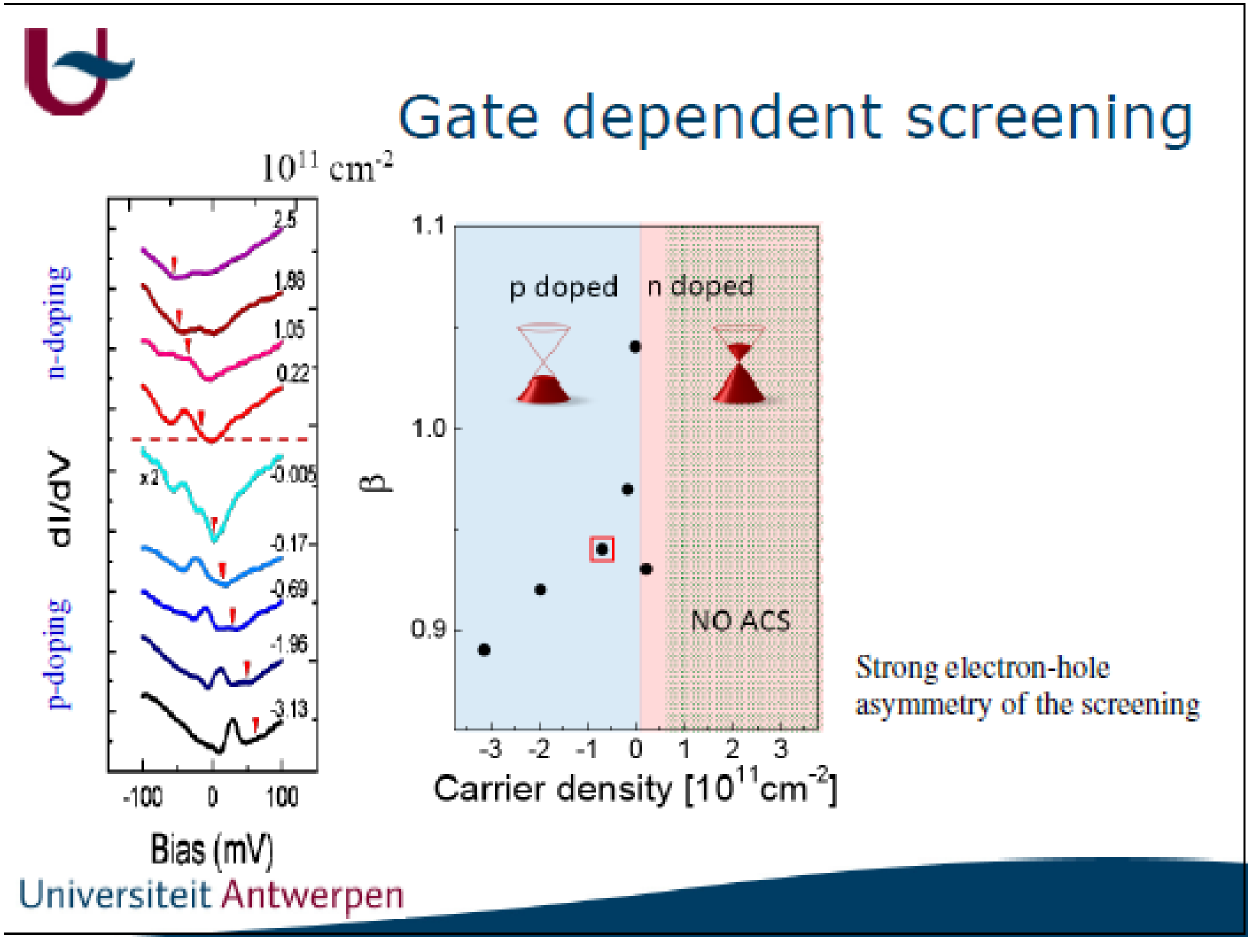

Gate dependent screening

Strong electron-hole asymmetry of the screening

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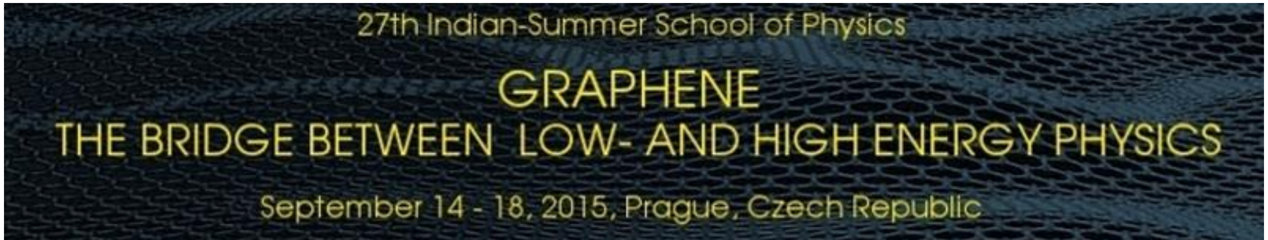

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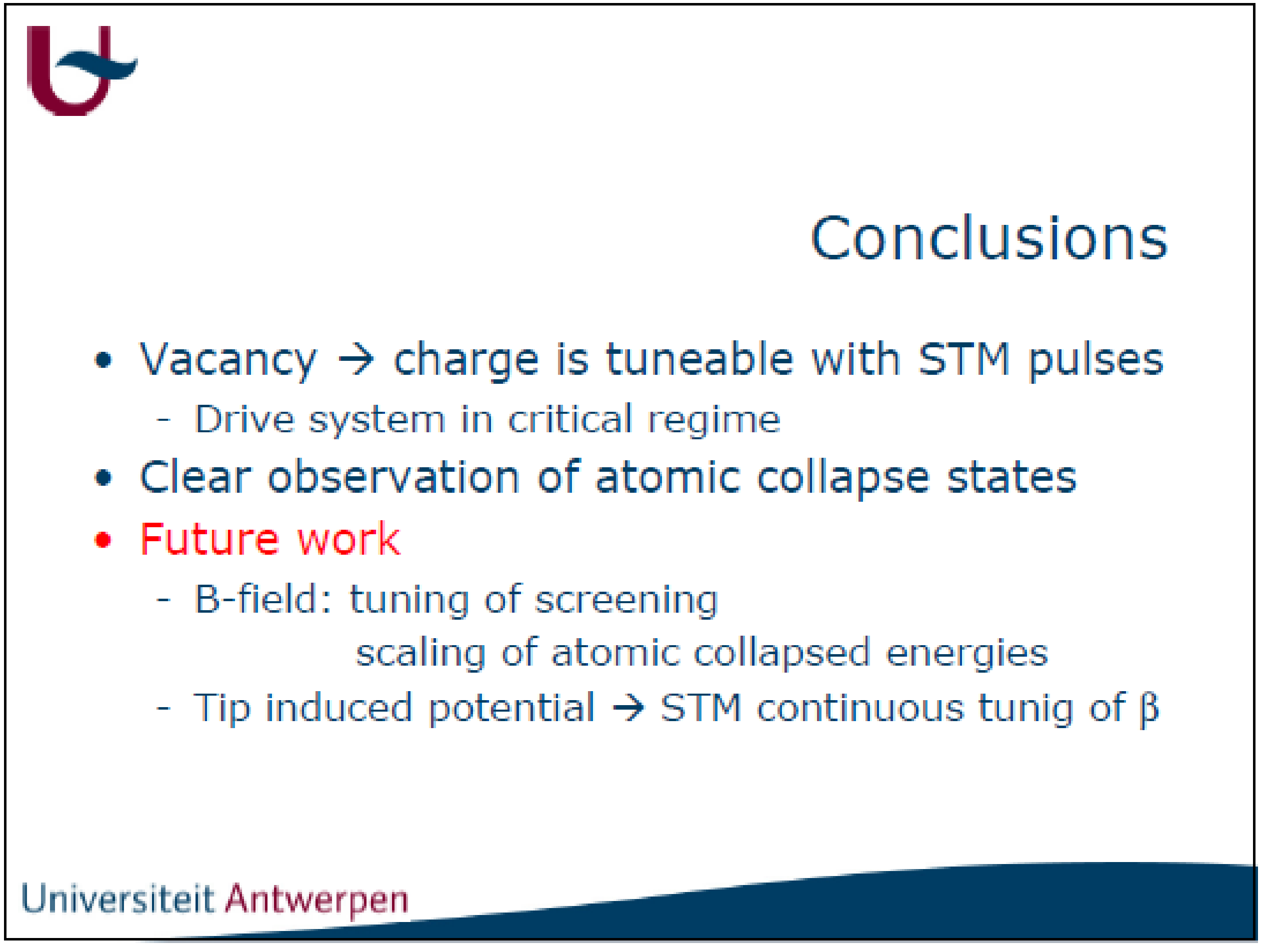
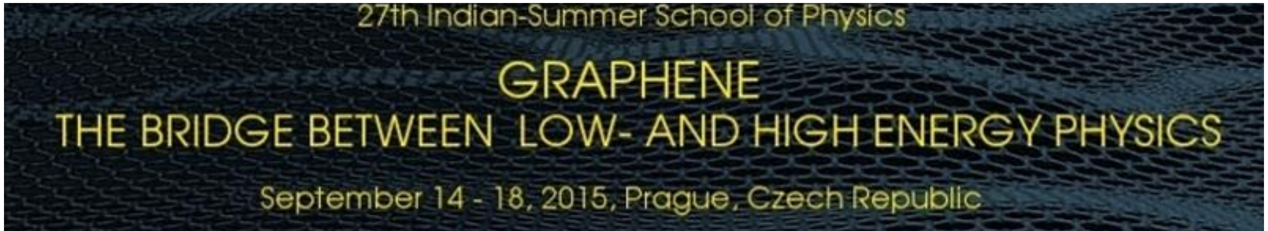


Conclusions

- Vacancy → charge is tuneable with STM pulses
  - Drive system in critical regime
- Clear observation of atomic collapse states
- Future work
  - B-field: tuning of screening
    scaling of atomic collapsed energies
  - Tip induced potential → STM continuous tunig of β

Universiteit Antwerpen



27th Indian-Summer School of Physics

GRAPHENE

THE BRIDGE BETWEEN LOW- AND HIGH ENERGY PHYSICS

September 14 - 18, 2015, Prague, Czech Republic

INFN is Scientific Partner in EU project “Graphene-Based Revolutions in ICT And Beyond, **GRAPHENE** Flagship

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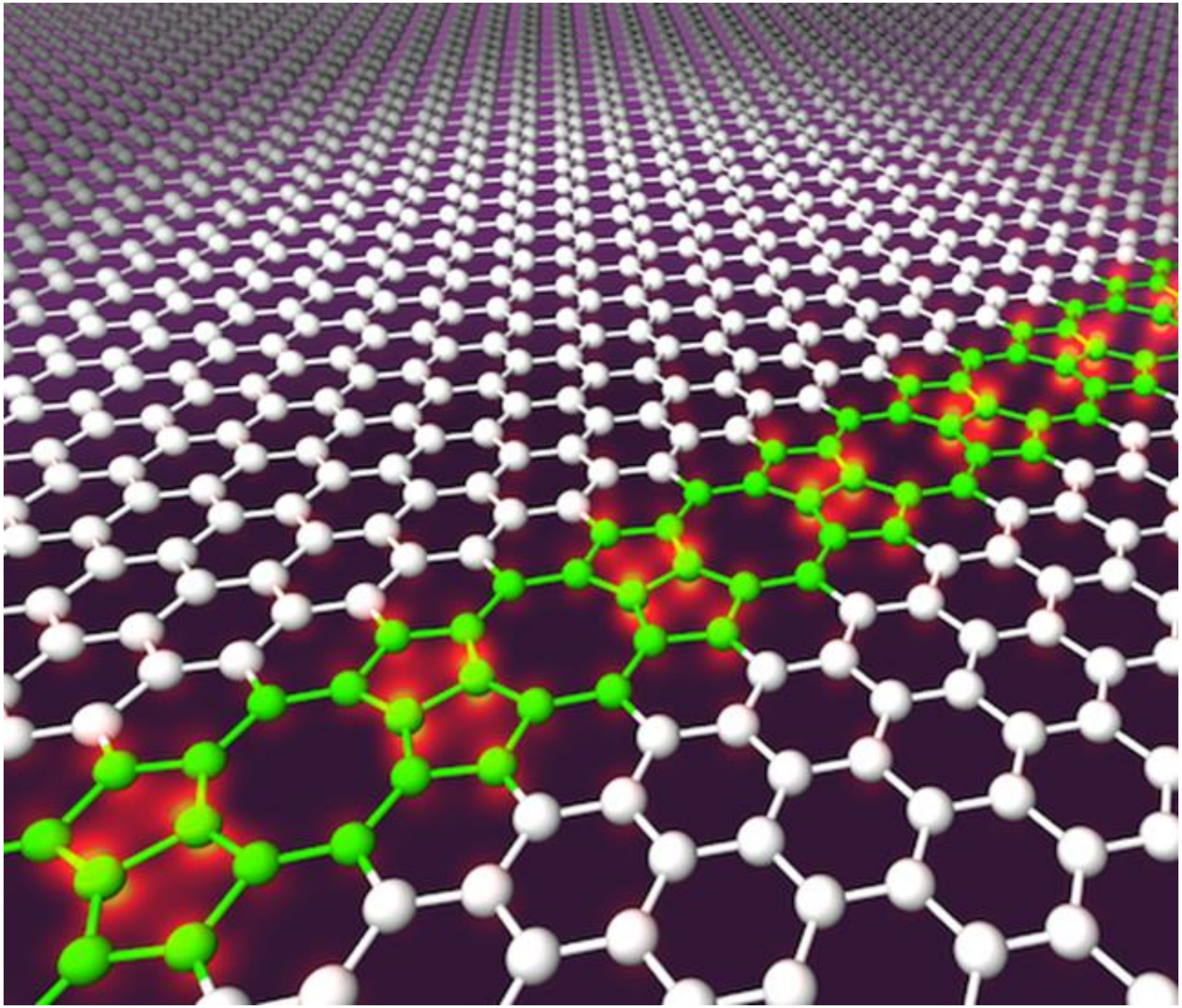
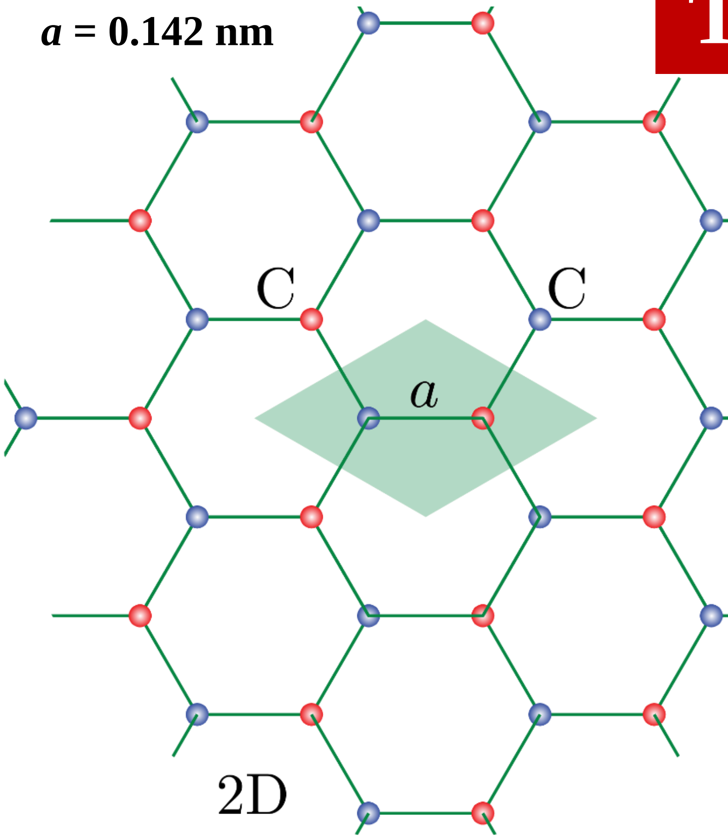
Graphene and Graphene NanoRibbons



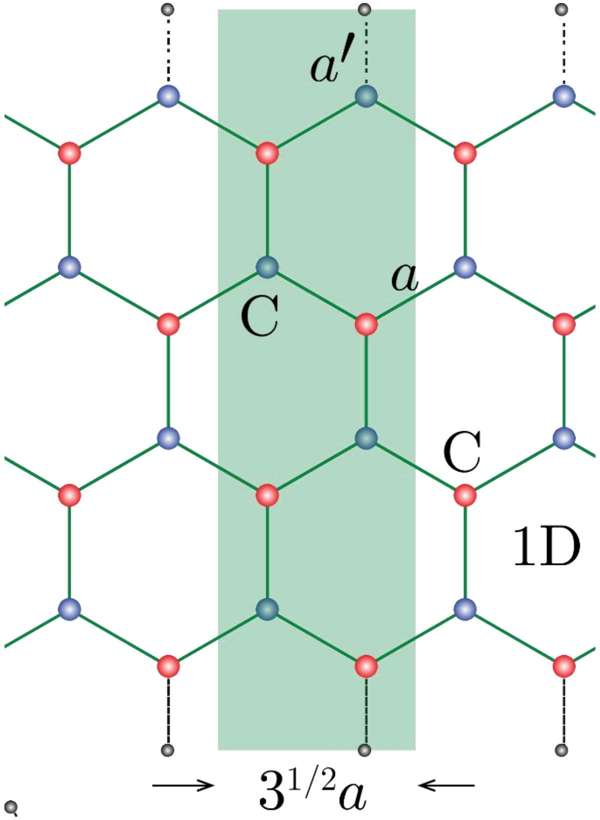
An Electromagnetic Characterization through the eyes of Linear Response Density Functional Theory

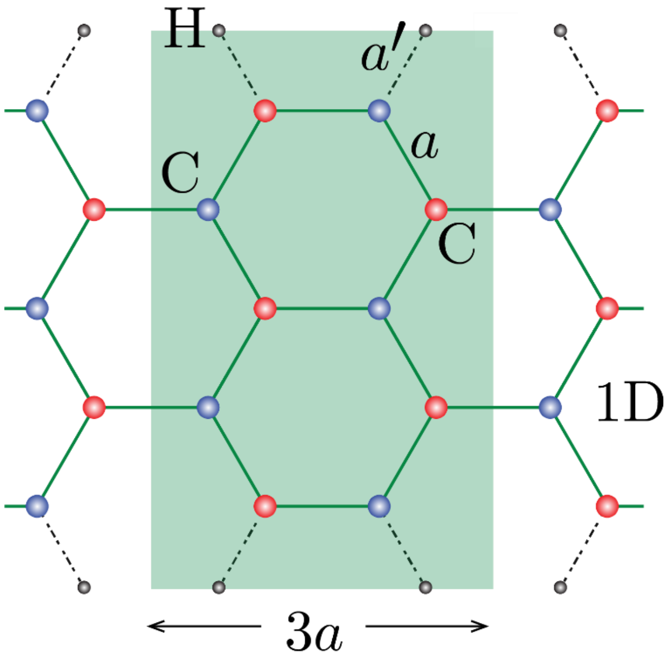
The Geometry

a **= 0.142 nm**



An ideal Graphene Sheet….

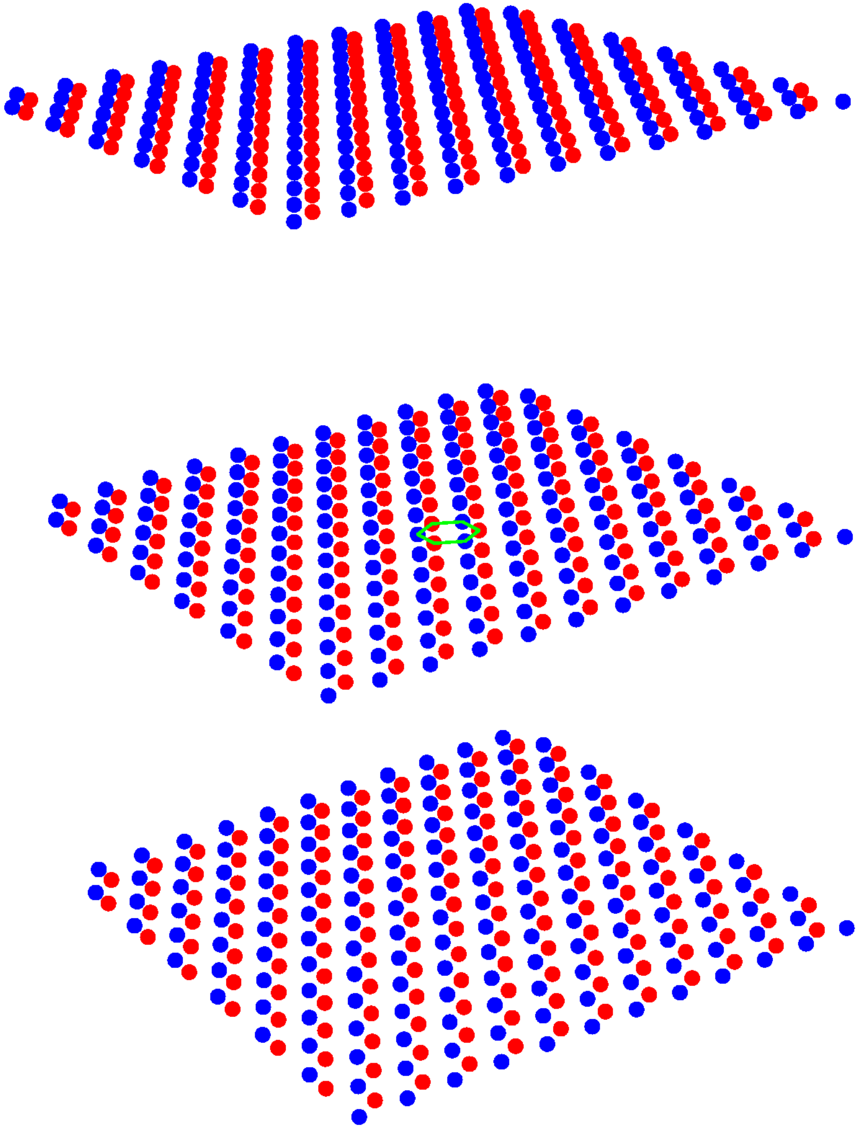




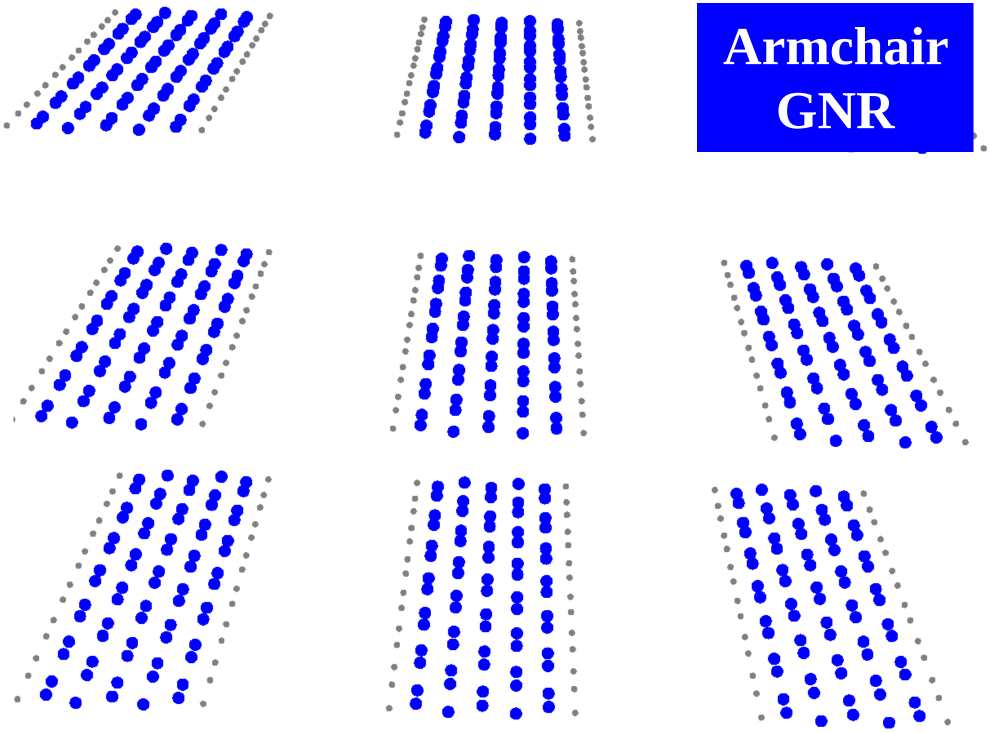
a **= 0.142 nm**
a' **= 0.1 nm**

… and two simple Armchair and Zig-Zag Graphene Ribbons (Edges passivated by Hydrogen atoms)

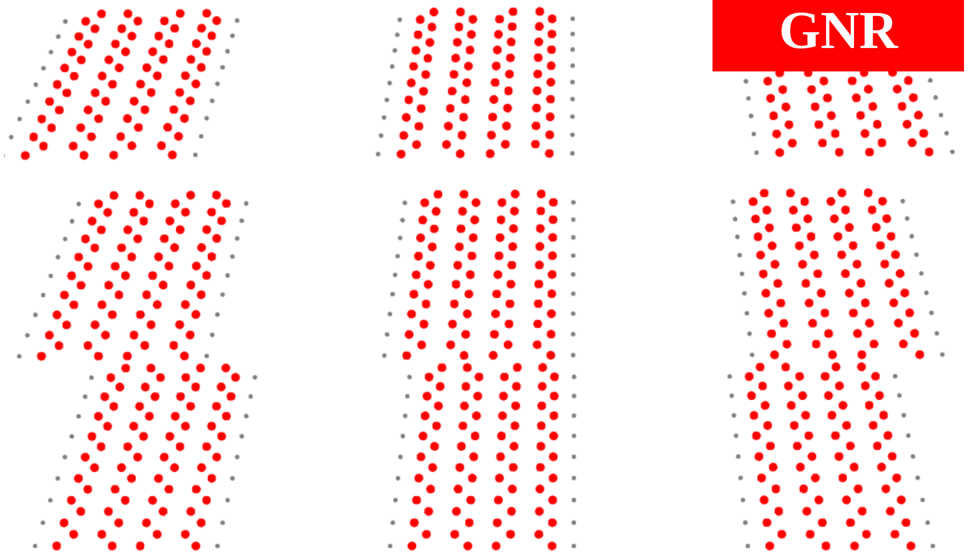
Imagine we replicate the structures and obtain the following 3D Crystals



Graphene



Armchair GNR

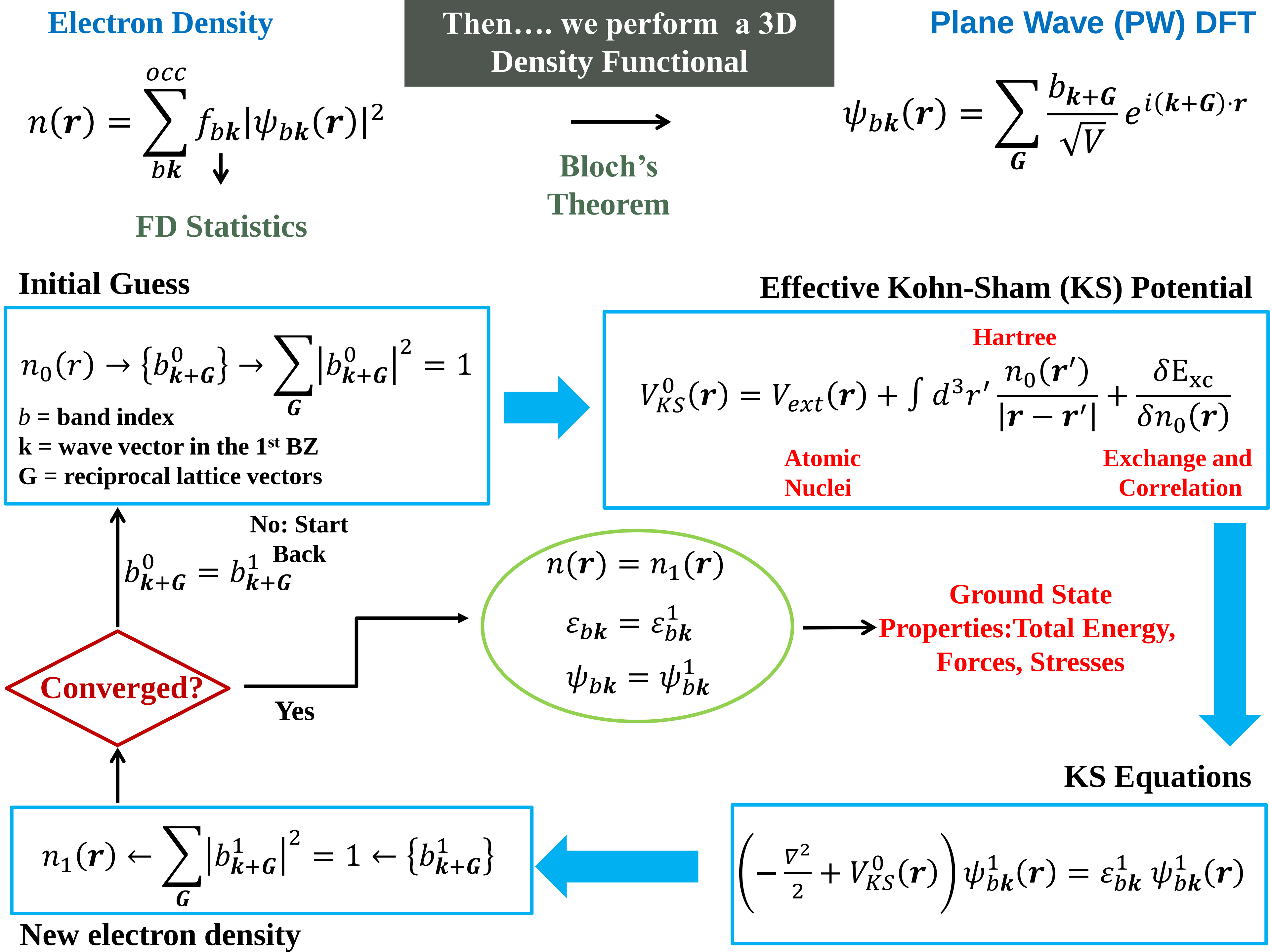


Zig-Zag GNR

Electron Density

Then…. we perform a 3D Density Functional

Plane Wave (PW) DFT



$$n(\boldsymbol{r}) = \sum_{b\boldsymbol{k}}^{occ} f_{b\boldsymbol{k}} |\psi_{b\boldsymbol{k}}(\boldsymbol{r})|^2$$

FD Statistics

$$\longrightarrow$$

Bloch's Theorem

$$\psi_{b\boldsymbol{k}}(\boldsymbol{r}) = \sum_{\boldsymbol{G}} \frac{b_{\boldsymbol{k}+\boldsymbol{G}}}{\sqrt{V}} e^{i(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{r}}$$

Initial Guess

$$n_0(r) \rightarrow \{b^0_{\boldsymbol{k}+\boldsymbol{G}}\} \rightarrow \sum_{\boldsymbol{G}} \left|b^0_{\boldsymbol{k}+\boldsymbol{G}}\right|^2 = 1$$

b = band index

k = wave vector in the 1st BZ

G = reciprocal lattice vectors

Effective Kohn-Sham (KS) Potential

Hartree

$$V^0_{KS}(\boldsymbol{r}) = V_{ext}(\boldsymbol{r}) + \int d^3r' \frac{n_0(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} + \frac{\delta \mathrm{E_{xc}}}{\delta n_0(\boldsymbol{r})}$$

Atomic Nuclei

Exchange and Correlation

KS Equations

$$\left(-\frac{\nabla^2}{2} + V^0_{KS}(\boldsymbol{r})\right)\psi^1_{b\boldsymbol{k}}(\boldsymbol{r}) = \varepsilon^1_{b\boldsymbol{k}}\, \psi^1_{b\boldsymbol{k}}(\boldsymbol{r})$$

New electron density

$$n_1(\boldsymbol{r}) \leftarrow \sum_{\boldsymbol{G}} \left|b^1_{\boldsymbol{k}+\boldsymbol{G}}\right|^2 = 1 \leftarrow \{b^1_{\boldsymbol{k}+\boldsymbol{G}}\}$$

Converged?

No: Start Back

$$b^0_{\boldsymbol{k}+\boldsymbol{G}} = b^1_{\boldsymbol{k}+\boldsymbol{G}}$$

Yes

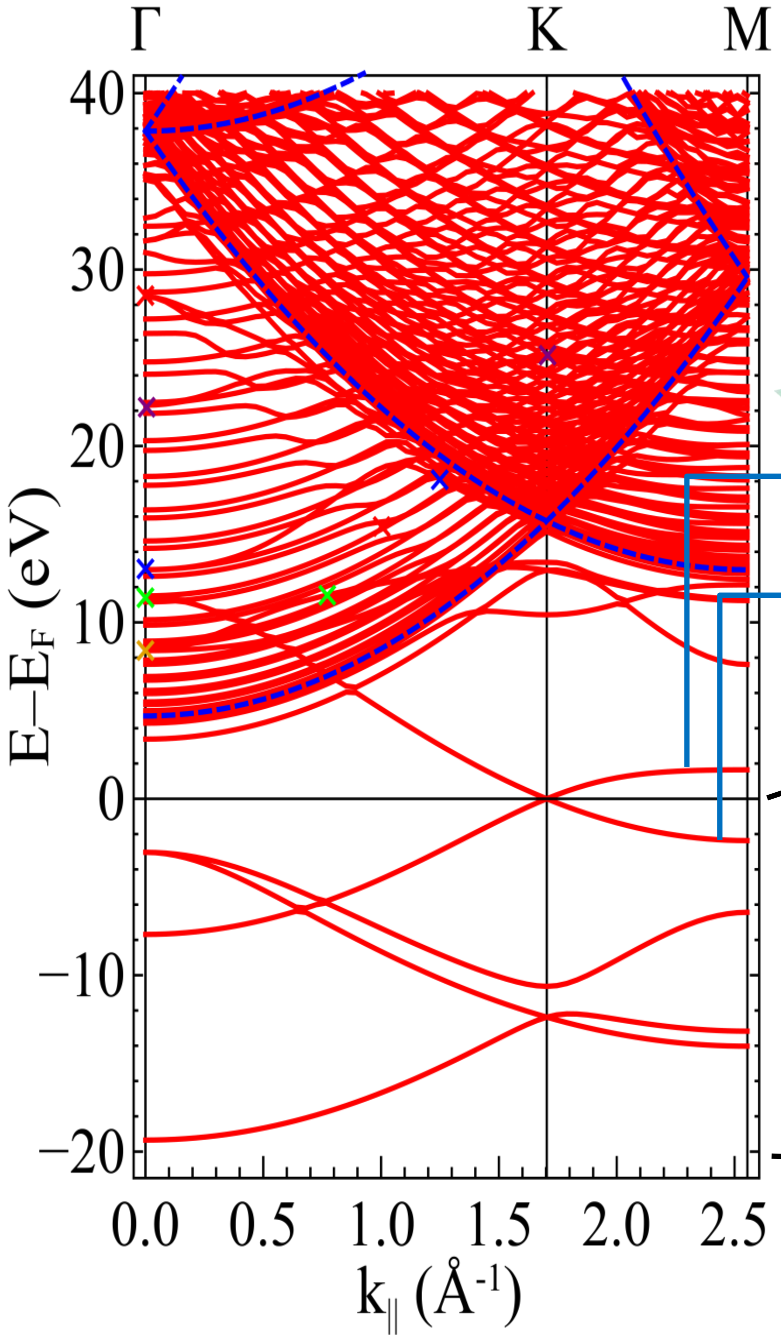
$$n(\boldsymbol{r}) = n_1(\boldsymbol{r})$$

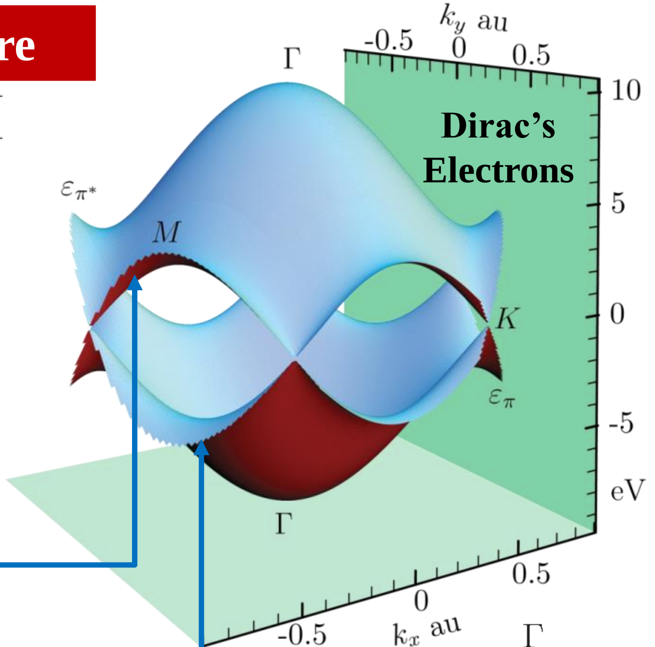
$$\varepsilon_{b\boldsymbol{k}} = \varepsilon^1_{b\boldsymbol{k}}$$

$$\psi_{b\boldsymbol{k}} = \psi^1_{b\boldsymbol{k}}$$

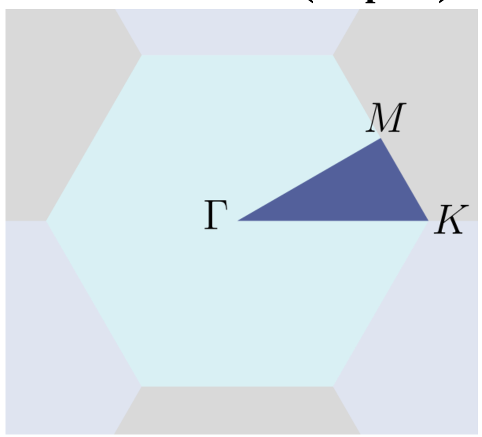
Ground State Properties:Total Energy, Forces, Stresses

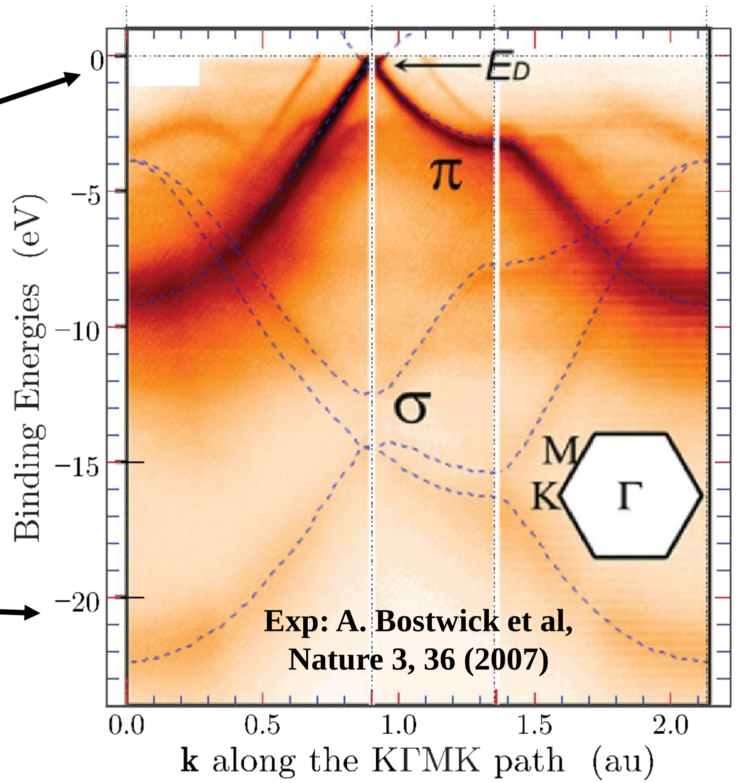
Graphene: Full electronic structure





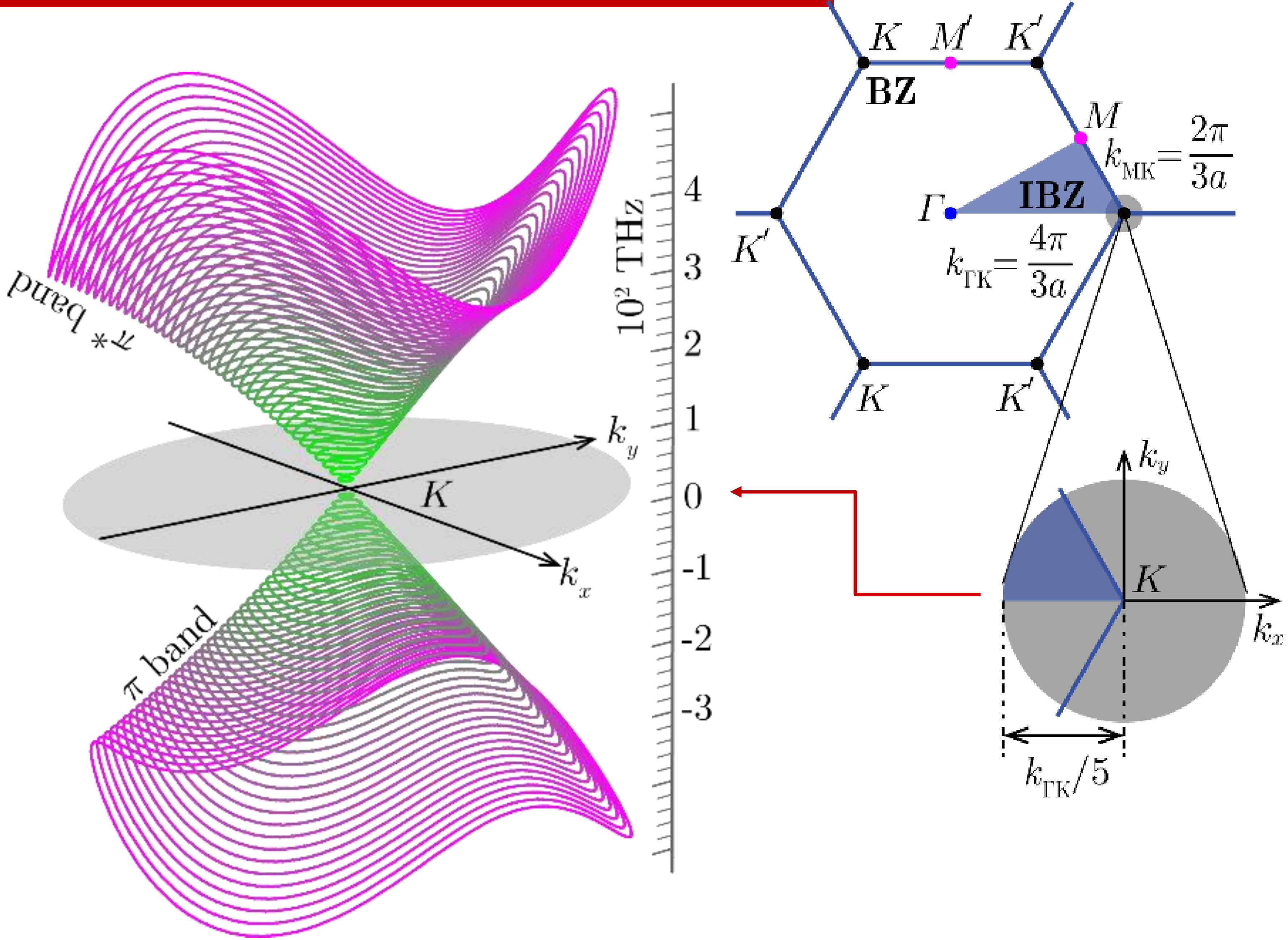
Brillouin ZONE (k Space)



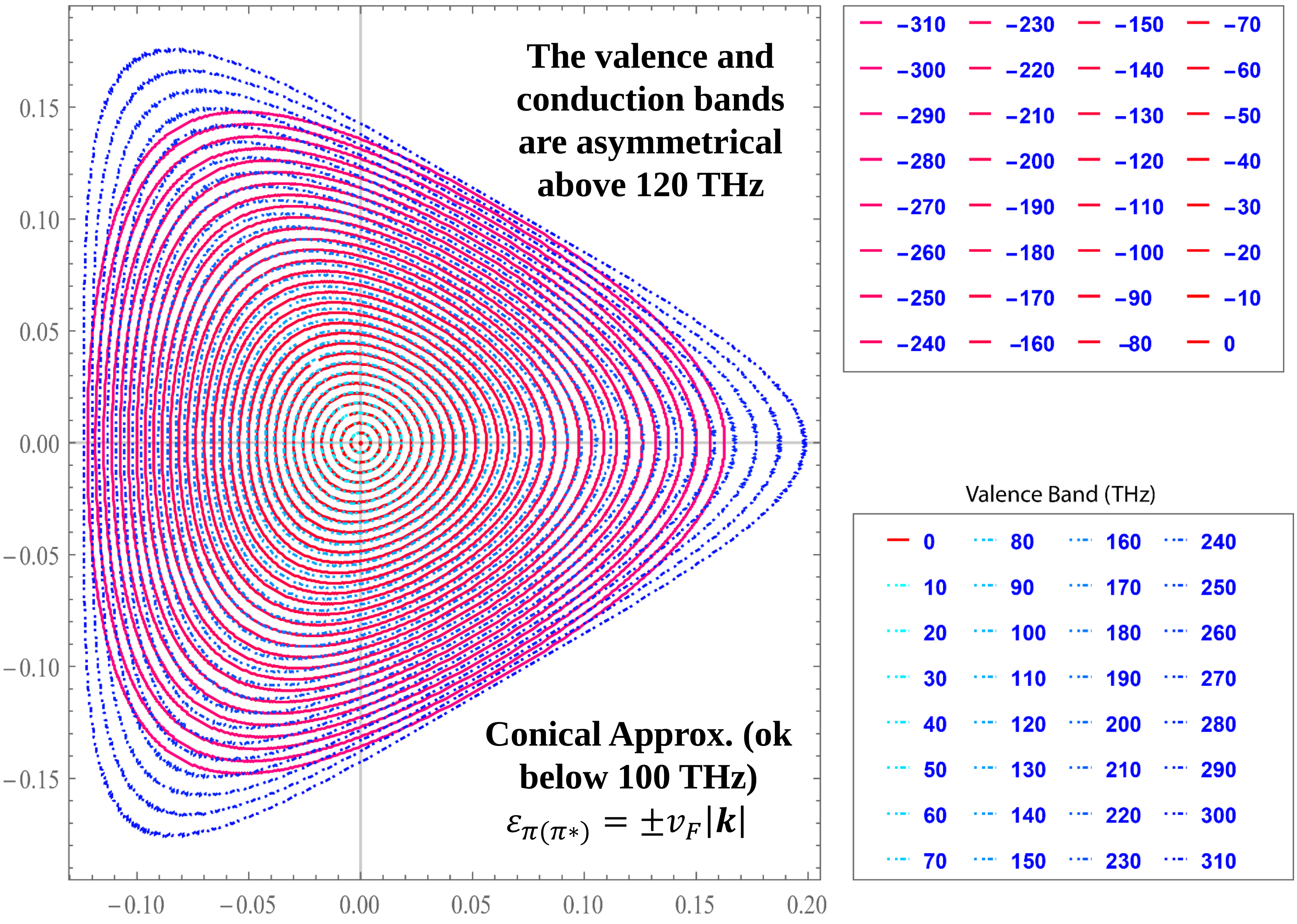


Exp: A. Bostwick et al, Nature 3, 36 (2007)

Graphene…zooming at the Dirac points (on the THz Scale)



Graphene…zooming at the Dirac points (on the THz Scale)



The valence and conduction bands are asymmetrical above 120 THz

Conical Approx. (ok below 100 THz)

$$\varepsilon_{\pi(\pi*)} = \pm v_F |\boldsymbol{k}|$$

Time Dependent DFT (Linear Response, RPA)

- Consider applying a small external electric field of wave-vector **q** and frequency ν
- The electric **displacement** and **conduction current** responses to the probing field are controlled by the **permittivity** and **conductivity** matrices

$$\epsilon_{\mathbf{GG}'}(\mathbf{q},\nu_{\pm}) = \epsilon_0 \delta_{\mathbf{GG}'} - \epsilon_0 \sum_{\boldsymbol{G}''} \boldsymbol{v}_{\boldsymbol{G}\boldsymbol{G}''}(\boldsymbol{q})\, \chi^0_{\boldsymbol{G}''\mathbf{G}'}(\mathbf{q},\nu_{\pm})$$

$$\sigma_{\mathbf{GG}'}(\mathbf{q},\nu_{\pm}) = ih\nu\epsilon_0 \sum_{\boldsymbol{G}''} \boldsymbol{v}_{\boldsymbol{G}\boldsymbol{G}''}(\boldsymbol{q})\, \chi^0_{\boldsymbol{G}''\mathbf{G}'}(\mathbf{q},\nu_{\pm})$$

DENSITY-DENSITY RESPONSE (LR THEORY)

$$\chi^0_{\boldsymbol{G}\mathbf{G}'}(\mathbf{q},\nu) = \frac{2}{\Omega} \sum_{\boldsymbol{k},n,n'} \frac{(f_{\varepsilon_{n\boldsymbol{k}}} - f_{\varepsilon_{n'\,\mathbf{k+q}}})\rho^{\mathbf{kq}}_{nn'}(\boldsymbol{G})\rho^{\mathbf{kq}}_{nn'}(\mathbf{G}')^*}{h\nu_{\pm} + \varepsilon_{n\boldsymbol{k}} - \varepsilon_{n'\,\boldsymbol{k+q}}}$$

All the basic ingredients, apart from τ (phenomenological relaxation time) that enters $\nu_{\pm} = \nu \pm j/\tau$, are computed by DFT, i.e.,

- the one-electron energies $\varepsilon_{n\boldsymbol{k}}$ and $\varepsilon_{n\mathbf{k+q}}$;
- the one-electron occupation factors $f_{\varepsilon_{n\mathbf{k}}}$ and $f_{\varepsilon_{n'\,\mathbf{k+q}}}$;
- the one-electron wave-functions $\psi_{n\mathbf{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{\Omega}}\sum_{\mathbf{G}} c_{n\mathbf{k+G}} e^{j(\mathbf{k+G})\cdot\mathbf{r}}$,
  - which appear in $\rho^{\mathbf{kq}}_{nn'}(\boldsymbol{G}) = \sum_{\mathbf{G}'''} \mathrm{c}^*_{n\mathbf{k+G}'}\, \mathrm{c}_{n'\mathbf{k+q}+\boldsymbol{G}+\mathbf{G}'}$;

The electron-electron interaction ($\boldsymbol{v}_{\boldsymbol{G}\boldsymbol{G}'}$ in reciprocal space) is part of the TD extension of DFT

Time Dependent DFT (Linear Response- 3D Coulomb Potential)

- Consider applying a small external electric field of wave-vector **q** and frequency ν
- The electric **displacement** and **conduction current** responses to the probing field are controlled by the **permittivity** and **conductivity** matrices

$$\epsilon_{\mathbf{GG}'}(\mathbf{q},\nu) = \epsilon_0\delta_{\mathbf{GG}'} - \sum_{\boldsymbol{G}''}\sum_{\boldsymbol{k}}\sum_{n,n'} \frac{\epsilon_0 v_{\boldsymbol{GG}''}(\boldsymbol{q})}{\Omega} \frac{\rho^{\mathbf{kq}}_{nn'}(\boldsymbol{G}'')(f_{\varepsilon_{n\boldsymbol{k}}} - f_{\varepsilon_{n'\,\mathbf{k+q}}})\rho^{\mathbf{kq}}_{nn'}(\mathbf{G}')^*}{h\nu_\pm + \varepsilon_{n\boldsymbol{k}} - \varepsilon_{n'\,\boldsymbol{k+q}}}$$

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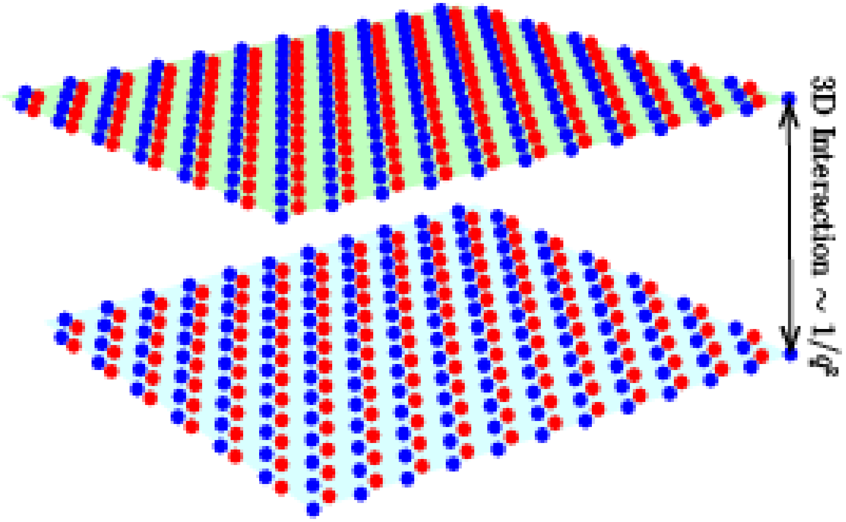
Electron-Electron interaction (3D)

$$v_{\boldsymbol{GG}'}(\boldsymbol{q}) = \frac{e^2\delta_{\mathbf{GG}'}}{\epsilon_0|\mathbf{q}+\mathbf{G}|^2}$$

$$\xrightarrow[\mathbf{G=G'=0}]{\textbf{Unwanted effect}}$$



Macroscopic Average

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

Resistivity Tensor $\rho_{\alpha\alpha}(q,\nu) = [\sigma_{\mathbf{GG}'}(q\boldsymbol{u}_\alpha,\nu)^{-1}]_{\mathbf{G=G}'=0}$

Time Dependent DFT (Linear Response- 3D Coulomb Potential)

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$$\sigma_{\mathbf{GG'}}(\mathbf{q},\nu) = ih\nu_{\pm} \sum_{\boldsymbol{G''}} \sum_{\boldsymbol{k}} \sum_{n,n'} \frac{\epsilon_0 v_{\boldsymbol{GG''}}(\boldsymbol{q})}{\Omega} \frac{\rho^{\mathbf{kq}}_{nn'}(\boldsymbol{G''})(f_{\varepsilon_{n\boldsymbol{k}}} - f_{\varepsilon_{n'\,\mathbf{k+q}}})\rho^{\mathbf{kq}}_{nn'}(\mathbf{G'})^*}{h\nu_{\pm} + \varepsilon_{n\boldsymbol{k}} - \varepsilon_{n'\,\boldsymbol{k+q}}}$$

Electron-Electron interaction (2D) …. **G**=(**g**,Gz) **and G'**=(**g'**,Gz')

$$v^{2D}_{\boldsymbol{GG'}}(\boldsymbol{q}) = v_{\boldsymbol{GG'}}(\boldsymbol{q}) - \frac{e^2\delta_{\boldsymbol{gg'}}}{\epsilon_0} \frac{1-e^{-L|\boldsymbol{q}+\boldsymbol{g}|}}{|\boldsymbol{q}+\boldsymbol{g}|L} \frac{|\boldsymbol{q}+\boldsymbol{g}|^2 - G_z G_z'}{(|\boldsymbol{q}+\boldsymbol{g}|^2 + G_z^2)(|\boldsymbol{q}+\boldsymbol{g}|^2 + G_z'^2)}$$

2D Cut-Off

$$\begin{matrix} G_z, G_z' \to 0 \\ \boldsymbol{g}, \boldsymbol{g}' \to 0 \end{matrix} \longrightarrow \frac{e^2 L}{2\epsilon_0 q}$$

The cut-off allows only in-plane electrons to interact with one another

Macroscopic Average

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

Resistivity Tensor $\rho_{\alpha\alpha}(q,\nu) = [\sigma_{\mathbf{GG'}}(q\boldsymbol{u}_\alpha,\nu)^{-1}]_{\mathbf{G}=\mathbf{G'}=0}$

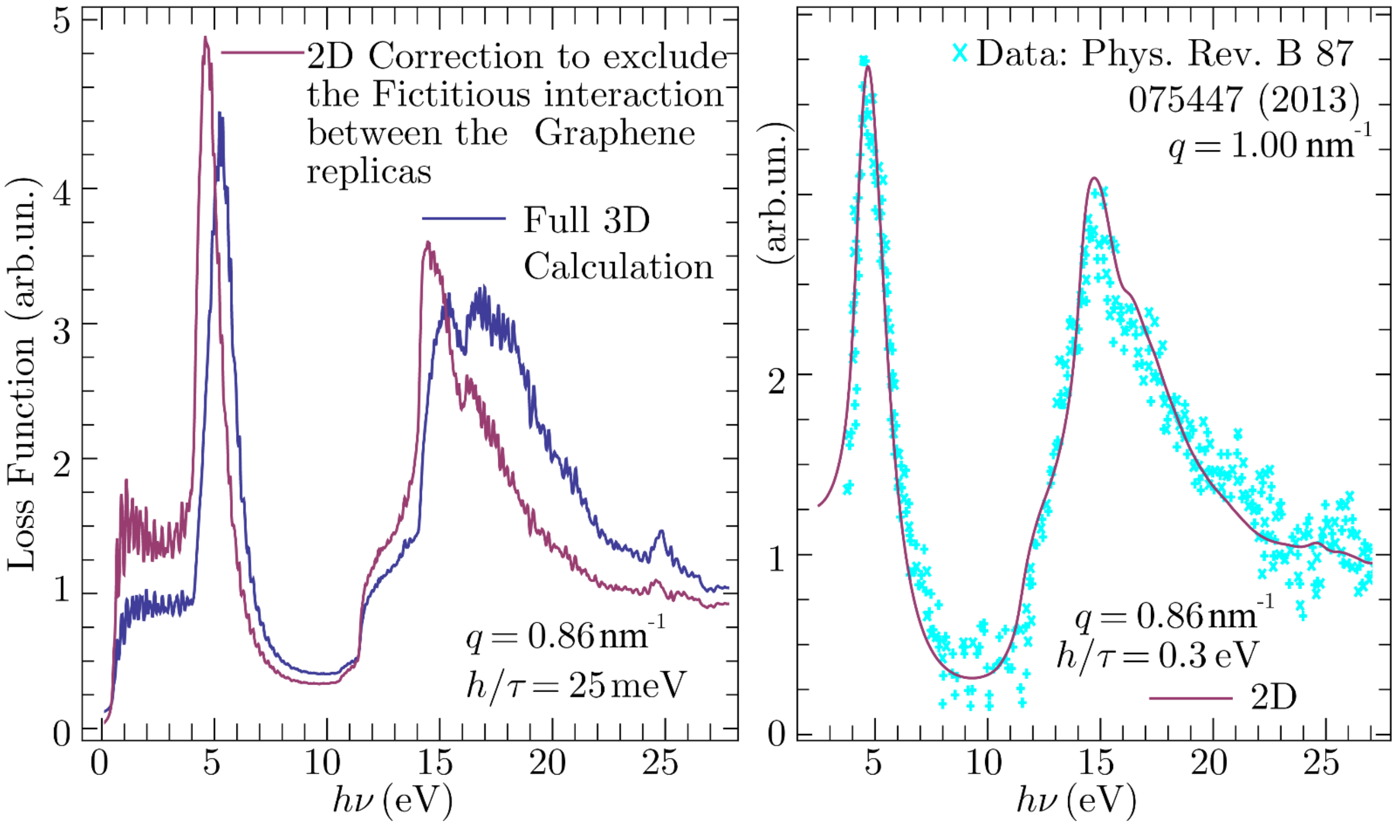
Observables

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

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

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

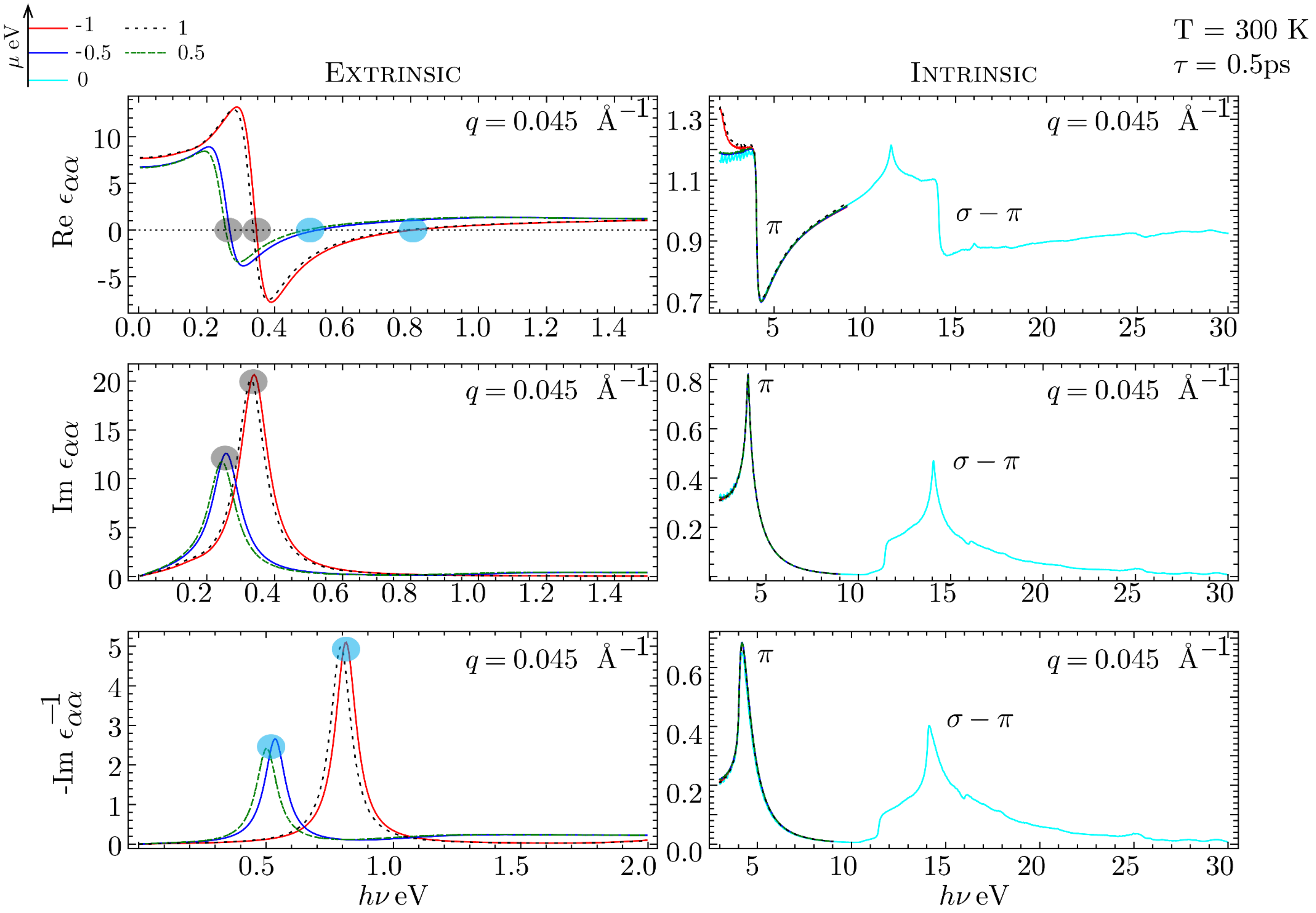
Application to Electron Energy Loss Data



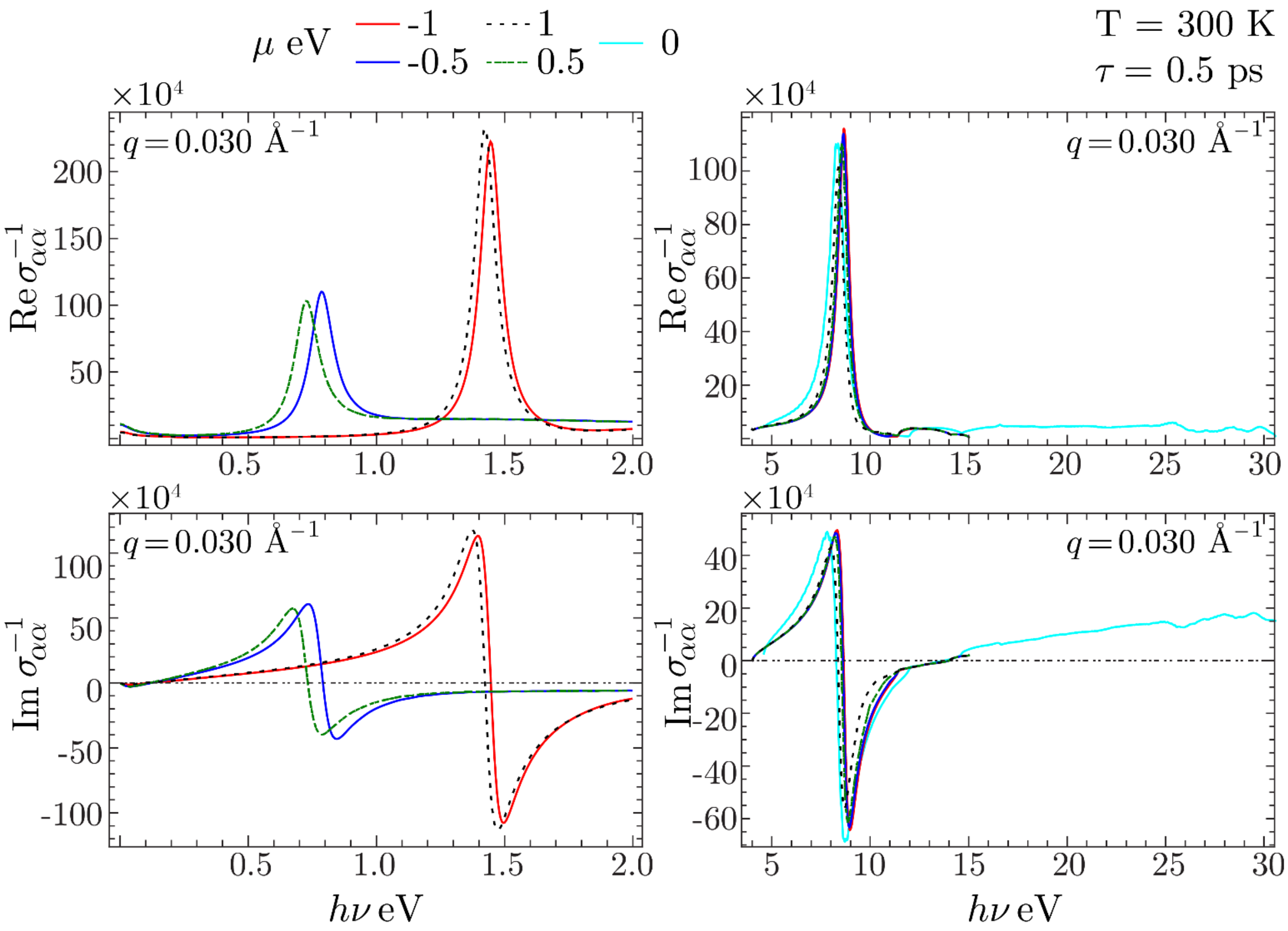
$L\,\mathrm{Re}[\rho_{\alpha\alpha}(q,\nu)]$ ↔ **Surface Resisistance**

$L\,\mathrm{Im}[\rho_{\alpha\alpha}(q,\nu)]$ ↔ **Surface Reactance**

Permittivity (Room T)



Resistivity (Room T)



Dirac-Cone Approximation & Optical Limit

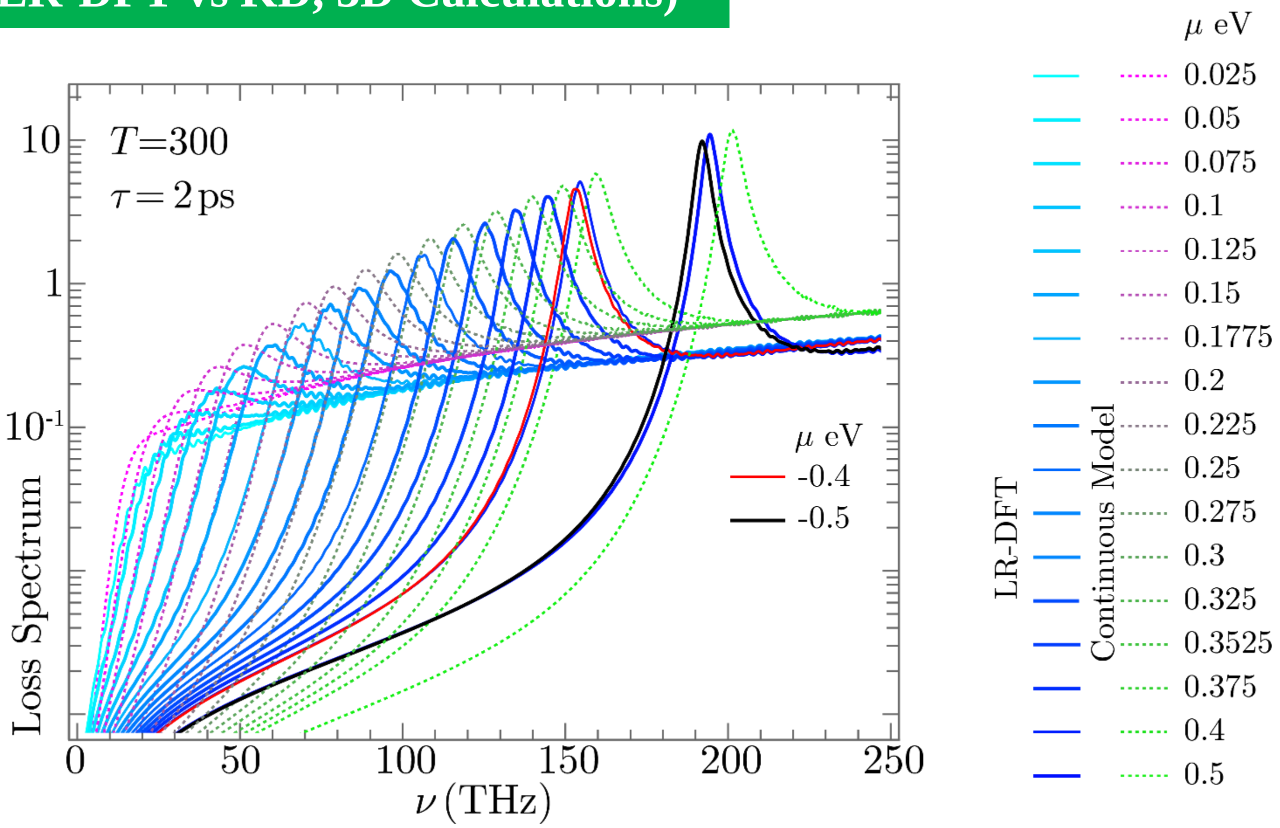
$$\epsilon_{\alpha\alpha}(q \to 0, \nu_{\pm}) = \epsilon_0 - \frac{e^2}{L\pi}\int_0^{\infty} \frac{d\varepsilon}{h^2\nu_{\pm}^2}\left(\varepsilon\frac{\partial}{\partial\varepsilon} + \frac{1}{h^2\nu_{\pm}^2 - 4\varepsilon^2}\right)(f_{\varepsilon} - f_{-\varepsilon})$$

Kubo-Drude Formula

$$\nu_{\pm} = \nu \pm \frac{i}{\tau}$$

$$\sigma_{\alpha\alpha}(q \to 0, \omega_{\pm}) = \frac{je^2}{\pi\hbar\, L}\int_0^{\infty} \frac{d\varepsilon}{h\nu_{\pm}}\left(\varepsilon\frac{\partial}{\partial\varepsilon} + \frac{h^2\nu_{\pm}^2}{h^2\nu_{\pm}^2 - 4\varepsilon^2}\right)(f_{\varepsilon} - f_{-\varepsilon})$$

Permittivity (LR-DFT vs KD, 3D Calculations)



Dirac-Cone Approximation & Optical Limit

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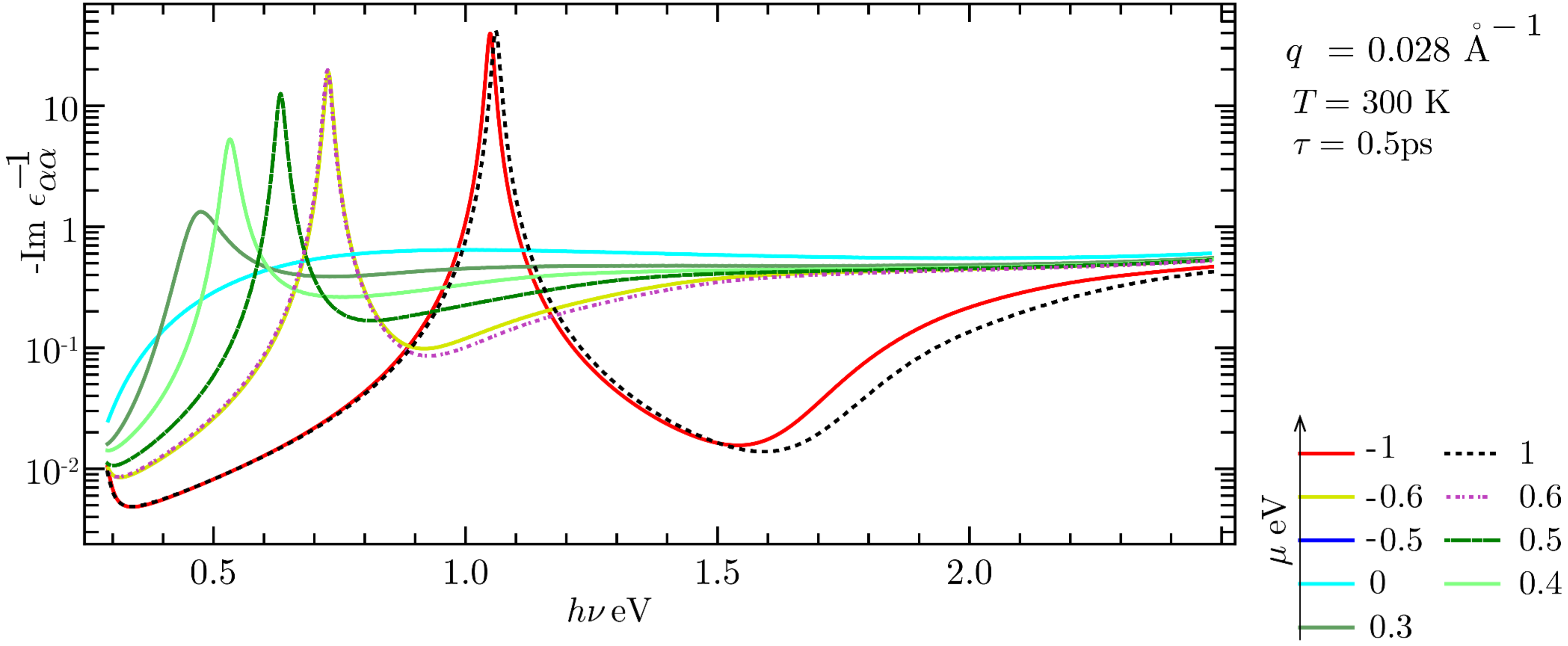
Permittivity (LR-DFT, 2D Calculations)



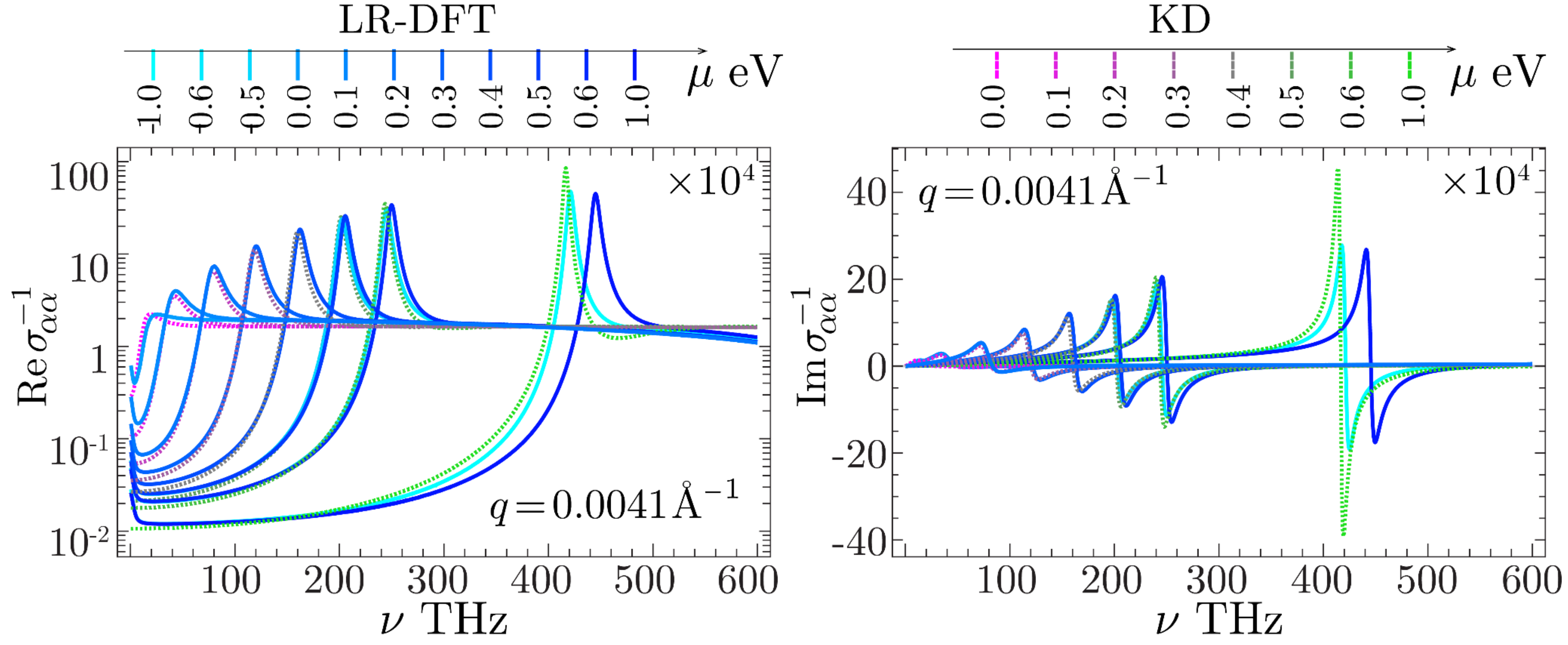
Conductivity-Resistivity (LR-DFT vs KD)

Kubo-Drude Formula

$$\sigma_{\alpha\alpha}(q \to 0, \omega_{\pm}) = \frac{je^2}{\pi\hbar\, L}\int_0^{\infty} \frac{d\varepsilon}{h\nu_{\pm}}\left(\varepsilon\frac{\partial}{\partial\varepsilon} + \frac{h^2\nu_{\pm}^2}{h^2\nu_{\pm}^2 - 4\varepsilon^2}\right)(f_{\varepsilon} - f_{-\varepsilon})$$

LR-DFT

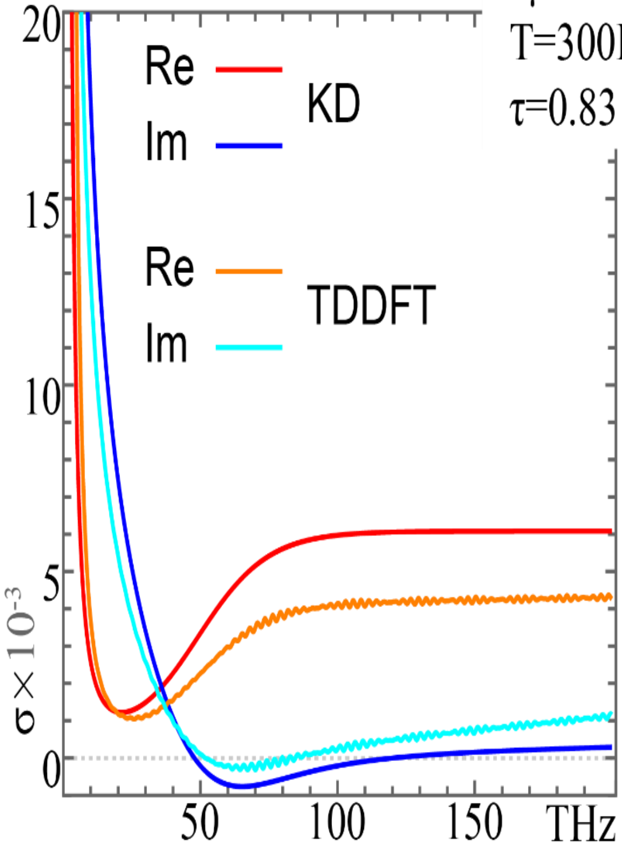
$$\sigma_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\nu\,) = ih\nu_{\pm}\sum_{\boldsymbol{G}''}\sum_{\boldsymbol{k}}\sum_{n,n'}\frac{\epsilon_0 v_{\boldsymbol{G}\boldsymbol{G}''}(\boldsymbol{q})}{\Omega}\frac{\rho_{nn'}^{\mathbf{kq}}(\boldsymbol{G}'')(f_{\varepsilon_{n\boldsymbol{k}}} - f_{\varepsilon_{n'\,\mathbf{k+q}}})\rho_{nn'}^{\mathbf{kq}}(\mathbf{G}')^*}{h\nu_{\pm} + \varepsilon_{n\boldsymbol{k}} - \varepsilon_{n'\,\boldsymbol{k+q}}}$$



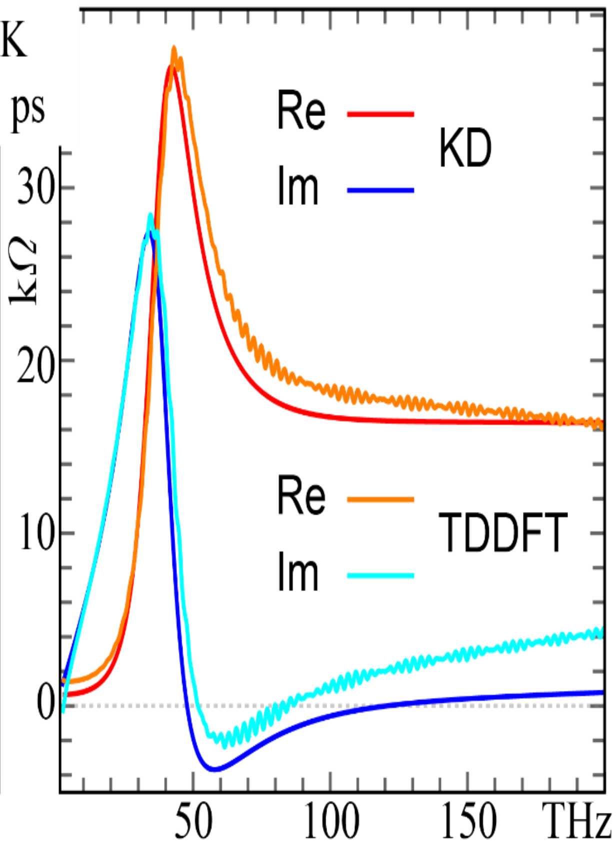
Conductivity vs Frequency

$\sigma_{\alpha\alpha}(q \rightarrow 0, \nu)$

δμ=0.1eV
T=300K
τ=0.83 ps

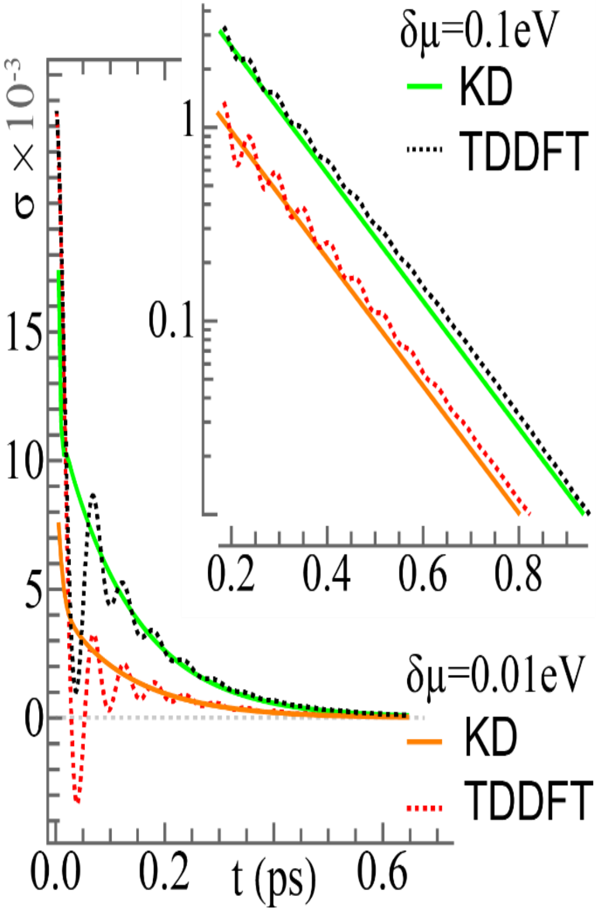


$\rho_{\alpha\alpha}(q \rightarrow 0, \nu)$



Conductivity vs Time

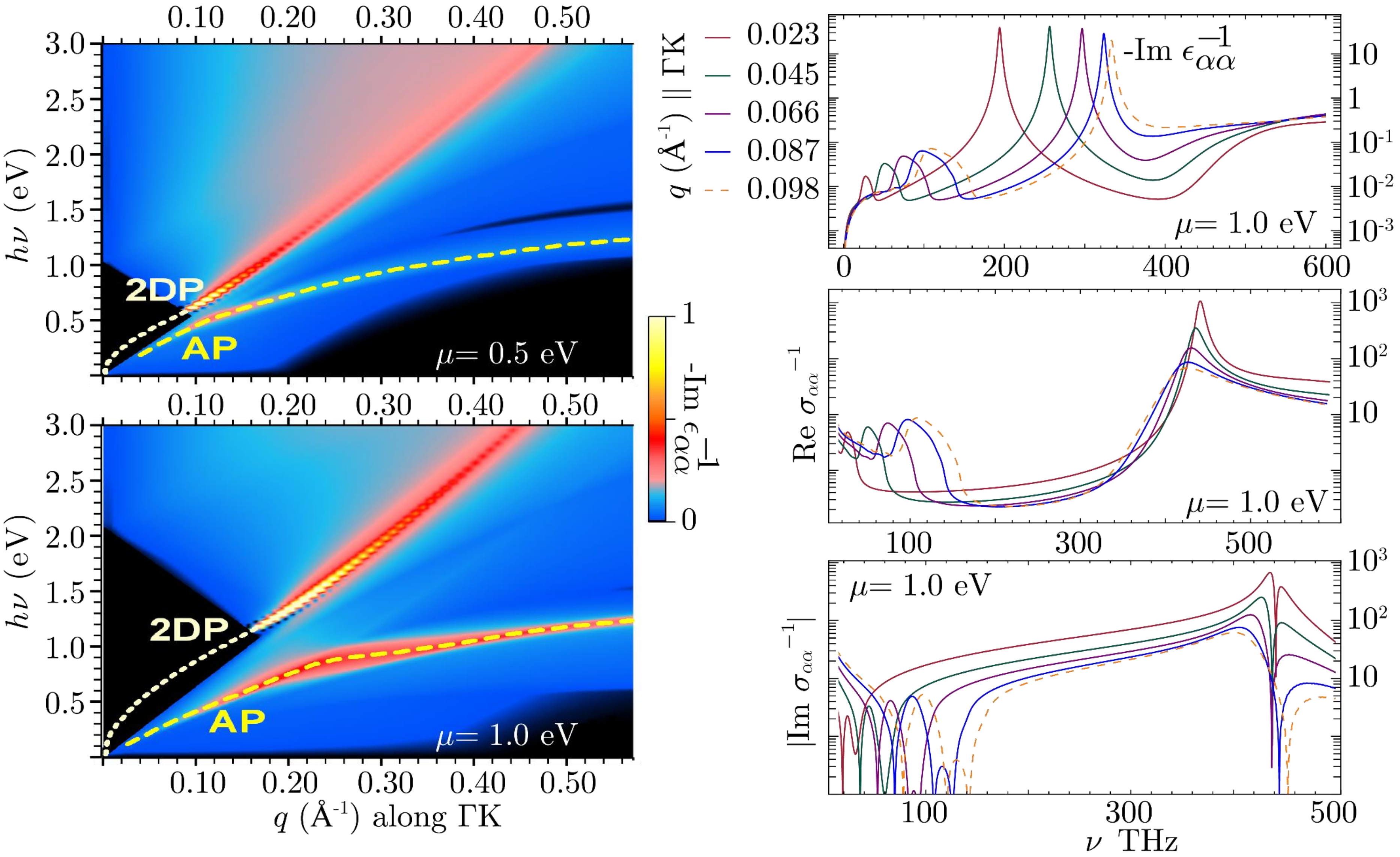
$\sigma_{\alpha\alpha}(q \rightarrow 0, t)$



Resisitvity vs Frequency

Acoustic Plasmon (?)

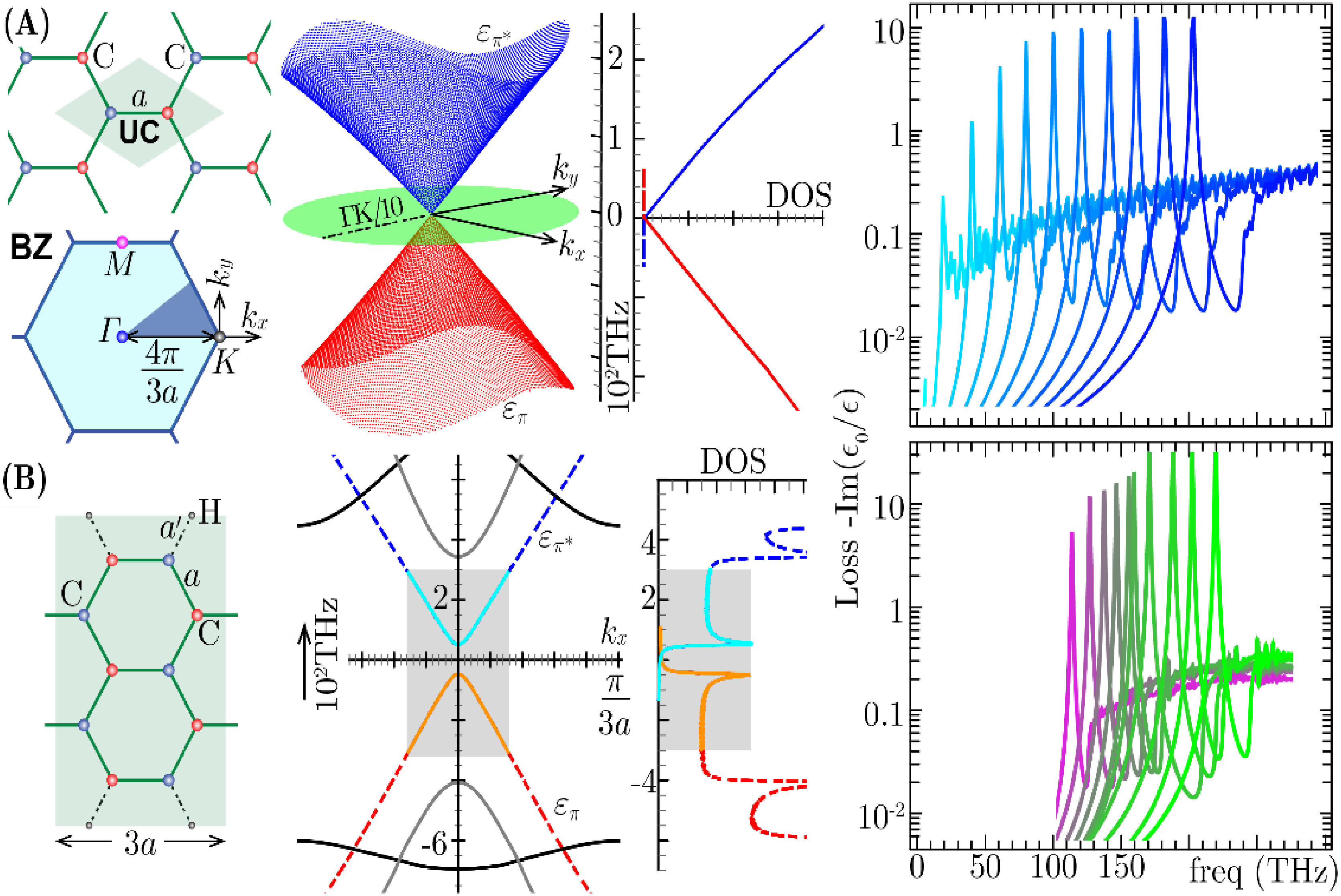
The two modes of collective oscillation due to coexistence of carriers moving with two distinct Fermi velocities:



(i) in one mode~(2DP) the two types of carriers oscillate in phase with one another (conventional 2D plasmon)

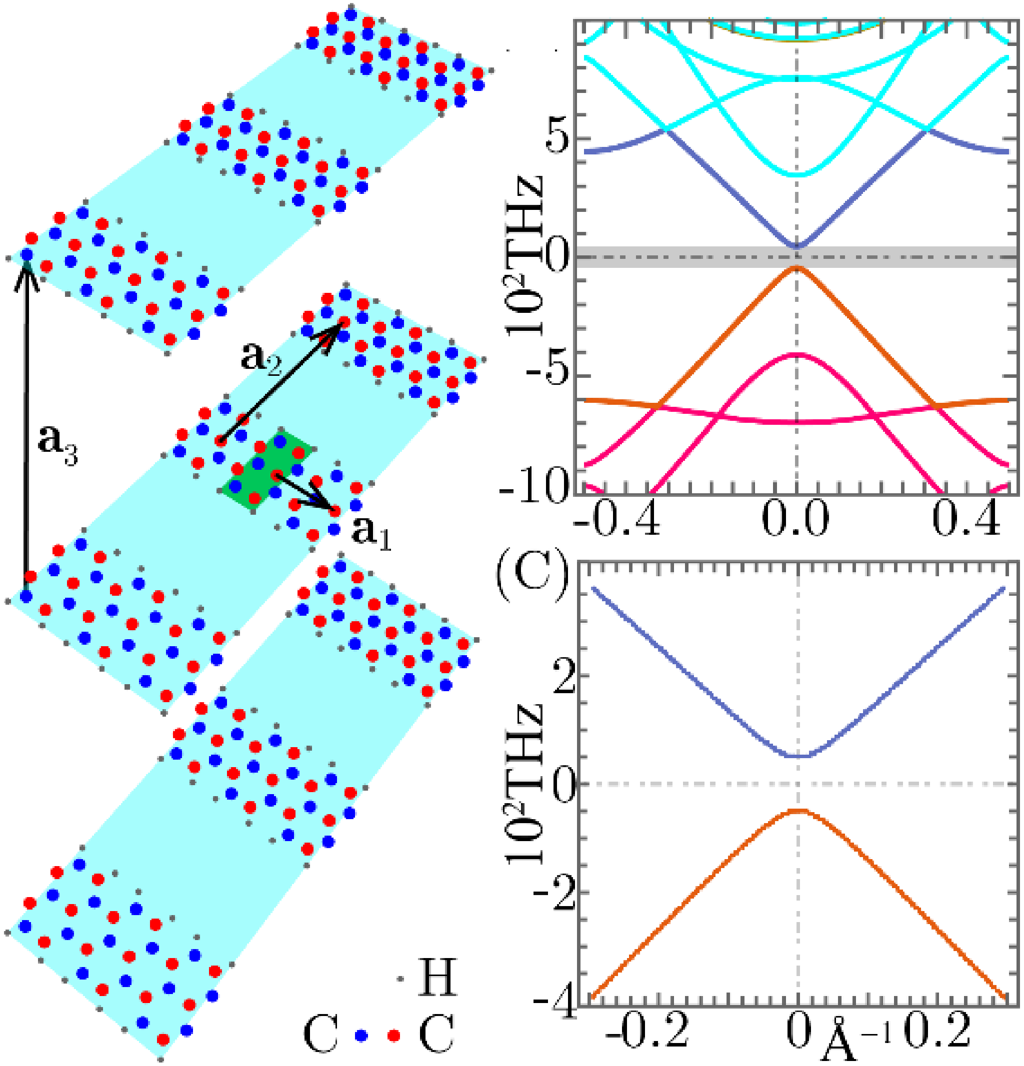
(ii) in the other mode~(AP) an acoustic is predicted to occur with the two types of carriers oscillating out of phase.

Permittivity response of graphene vs an armchair nanoribbon



Only LR-DFT can be used (no conical approx.)

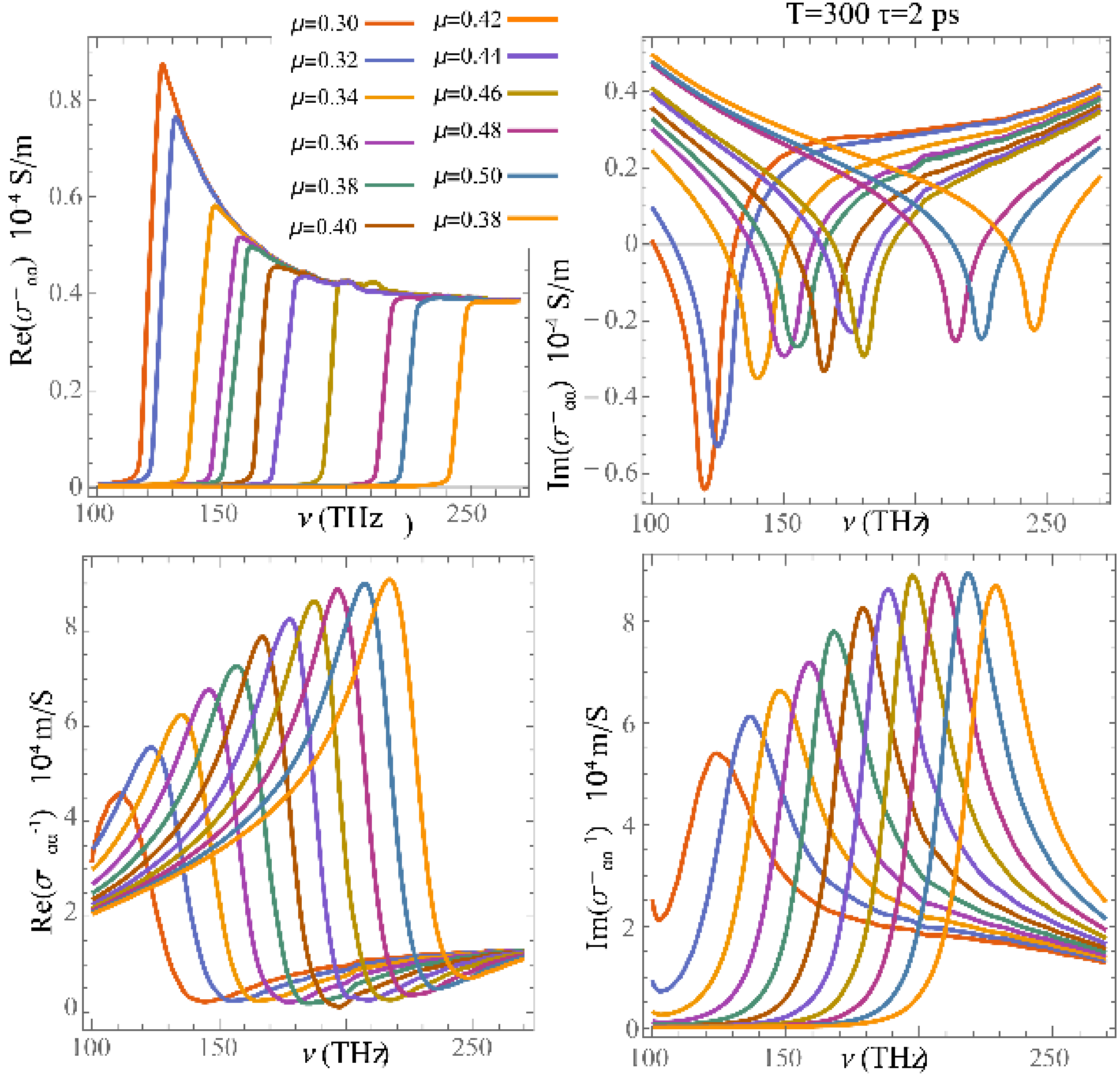
Armchair nanoribbon (5,5)



Real space geometry, band structure, and dispersion relations for the π and π^* electronic bands in a pristine (5,5) GNR

Only LR-DFT can be used (no conical approx.)

Armchair nanoribbon (5,5) -> Conductivity/Resistivity



Only LR-DFT can be used (no conical approx.)

- We have presented advanced tools to study the linear electromagnetic response of graphene and graphene-like materials on the THz scale.
- Starting from an atomistic point of view, we have defined an ab initio approach in which the ground state properties of the material, i.e., energies, occupations, and one-electron wave-functions are computed by plane-wave DFT.
- These information are plugged in the relations of linear response theory to predict the EM response of the system, in the optical limit .
- Although several permittivity simulations have been performed, following similar guidelines, on pristine graphene on the eV scale, here we have defined a procedure to properly sample the electronic structure on the THz scale.
- At the same time, we have tested the reliability of the widely-used KD approach, operating in the same frequency range.
- Upon comparison of DFT-results with those obtained by the KD formulation, some significant differences have been pointed out. Nevertheless the KD formula seems to reasonably capture the main quantum features of graphene for EM applications. However, the proposed ab initio tool can be feasibly adapted to describe graphene-like systems with a more complex electronic structure than graphene, such as graphene multilayers, nano-ribbons, or nanotubes.
- More importantly, it has the potential to properly account for the role of metal contacts and substrate contacts. This is the object of current and future work.

INFN

NEXT

NANOTECHNOLOGY LABORATORIES

NANOSCIENCE EXPERIMENTS FOR TECHNOLOGY

Thanks for your attention!