

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

NEMESYS



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di Cosenza

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Prof. Francesco Plastina

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(Local Coordinator)

Prof. Olivia Pulci

Dr. Maurizia Palummo



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(Local Coordinator)

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Fundamental Physics and
Applications

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(Local Coordinator)

Dr. Maurizio Dapor

Dr. Giovanni Garberoglio



SAPIENZA
UNIVERSITÀ DI ROMA

Large Scale Computing @ INFN
13.02.2017

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

NEMESYS (2017-2020)



Dr. Antonello SINDONA*
(National Coordinator)



Dr. Stefano Bellucci
(Local Coordinator)



Dr. Gianluca Stefanucci
(Local Coordinator)



Dr. Simone Taioli
(Local Coordinator)

Previous Specific Initiatives (Parent Projects)

SEMS (2013-2016)



Dr. Stefano Bellucci
(National Coordinator)

LF61 (2004-2012)



Dr. Antonello SINDONA*
(Local Coordinator)

Aims and Scopes

- **Main theme.** 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,
 - ensembles of ultra-cold atomic gases,
 - magnetic and spin systems.
- **Program.** Massive simulations of
 - spectral features, dielectric screening, conductivity response and electro-mechanical properties of graphene-related and beyond-graphene materials, including their interfaces and contacts with supporting substrates
 - irreversible properties and quantum thermodynamics of ultra cold Fermi and Bose gases, following a change of their trapping potentials
- **Computational methods.**
 - Density Functional Theory (DFT) and Time Dependent (TD) extensions
 - Many Body Perturbation Theory
 - Topological quantum field theory on space-time (2+1) and (1+1) manifolds
 - Quantum Montecarlo
 - Semi classical Multiscale Approaches

Motivations

- **Fundamental properties**

- Dirac nature of the charge-carriers in honeycomb-like structures (massless electrons/positrons with energy $\varepsilon = \pm v_F |\mathbf{k}|$, $v_F \sim c/300$)
- Quantum Spin Hall Effect
- Calibration for universal constants (e.g., fine structure constant)
- Coherent charge-density fluctuations (plasmons)
- Nature of the many-body interaction in correlated many fermion systems (excitons, trions, biexcitons)
- Quantum phase transitions
- Entanglement content of many fermion and boson states
- Quantum thermodynamic transformations/cycles
- Bose–Einstein condensation (BEC)
- Bardeen-Cooper-Schrieffer (BCS) super fluidity and the BEC-BCS crossover
- Quantum magnetism and many-body spin dynamics

- **Systems**

- Graphene related nanostructures (nanotubes, nanoribbons, fullerenes)
- Beyond graphene materials (silicene, germanene, transition metal dichalcogenides)
- Atomic gases in mono(bi)-chromatic traps

Motivations

- **Technological Interests**

- Graphene, Graphyne, Borophene, Germanene, Silicene, Stanene, Phosphorene, Molybdenite, Graphane, Hexagonal Boron Nitride, Germanane, **Transition Metal Dichalcogenides**, MXenes, 3D-topological Structures are under close consideration for a number of industries, in areas including **electronics**, **optoelectronics**, **sensors**, biological engineering, filtration, photovoltaics, **medicine**, thermal management, energy storage
- Ultra cold atoms have been proposed as a platform for **quantum computation** and **quantum simulation**

- **Huge Investments**

- Graphene Flagship (Future and Emerging Technology Flagship by the European Commission, with a budget of €1 billion)
- Quantum technology Flagship (Future and Emerging Technology Flagship by the European Commission, with a budget of €1 billion)

- **Heavy Computational Demands**

- $\sim 10^5\text{-}10^6$ Core Hours per Simulation (DFT+TDDFT or DFT+GW)
- Big Data (0.1-1 TB per output file)

What are we good at...

- Parameter-free **Density Functional Theory** (DFT)
- **Time Dependent DFT** (TDDFT)
- **Many Body Perturbation Theory** (MBPT)
- **Green's Function** (GF) techniques

Selected Publications (2016-beginning 2017)

- Y. Pavlyukh, A. M. Uimonen, G. Stefanucci, R. van Leeuwen, "Vertex Corrections for Positive-Definite Spectral Functions of Simple Metals", **Physical Review Letters** 117, 206402 (2016)
- 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)
- A. Michele, K. Thanayut, A. Zobelli, M. Palummo, R. Rurali, "Crystal Phase Effects in Si Nanowire Polytypes and Their Homojunctions", **Nano Letters** 16, 5694 (2016)
- G. Francica, J. Goold, M. Paternostro, F. Plastina, "Daemonic Ergotropy: Enhanced Work Extraction from Quantum Correlations", **Nature Quantum Information** in Press (2017).
- A. Karlsson, F. Francica, J. Piilo, F. Plastina, "Quantum Zeno effect and non-Markovianity in a three-level system", **Scientific Reports** 6, 39061 (2016).
- L. A. Chernozatonskii, V. A. Demin, S. Bellucci, "Bilayered graphene/h-BN with folded holes as new nanoelectronic materials: modeling of structures and electronic properties", **Scientific Reports** 6, 38029 (2016)
- Y.B. Zhou, D.S. Fox, P. Maguire, R. O'Connell, R. Masters, C. Rodenburg, H.C. Wu, M. Dapor, Y. Chen, H. Z. Zhang, "Quantitative secondary electron imaging for work function extraction at atomic level and layer identification of graphene", **Scientific Reports** 6, 21045 (2016)
- M. Pisarra, A. Sindona, M. Gravina, V. M. Silkin and J. M. Pitarke, "Dielectric screening and plasmon resonances in bilayer graphene", **Physical Review B** 93, 035440 (2016)

INFN Referee Reports (2)

Quality and relevance of the proposed research activity: A A

Project feasibility, including methodology, research plan and strategy: A A

Project impact: A A

Research team qualification and role within the network: A A

Global evaluation: A A

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- S. Kurth, G. Stefanucci, "Nonequilibrium Anderson model made simple with density functional theory", **Physical Review B** 94(24), 241103 (2016)
- E. Perfetto, D. Sangalli, A. Marini, G. Stefanucci, "First-principles approach to excitons in time-resolved and angle-resolved photoemission spectra", **Physical Review B** 94(24), 245303 (2016)
- R. Tuovinen, N. Sakkinen, D. Karlsson, G. Stefanucci, R. van Leeuwen, "Phononic heat transport in the transient regime: An analytic solution", **Physical Review B** 93(21), 214301 (2016)
- K. Yang, E. Perfetto, S. Kurth, G. Stefanucci, R. D'Agosta, "Density functional theory of the Seebeck coefficient in the Coulomb blockade regime", **Physical Review B** 94(8), 081410 (2016)
- P. Riccardi, A. Sindona, C. A. Dukes, "Double electron excitation in He ions interacting with an aluminum surface", **Physical Review A** 93, 042710 (2016)
- S. Bellucci, A. A. Saharian, A. Kh. Grigoryan, "Induced fermionic charge and current densities in two-dimensional rings", **Physical Review D** 94, 105007 (2016)
- D. Mencarelli, L. Pierantoni, M. Stocchi, S. Bellucci, "Efficient and versatile graphene-based multilayers for EM field absorption", **Applied Physics Letters** 109(9), 093103 (2016)
- S. Bellucci, A. A. Saharian, V. Vardanyan, "Hadamard function and the vacuum currents in braneworlds with compact dimensions: Two-brane geometry", **Physical Review D** 93, 084011 (2016)

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Quality and relevance of the proposed research activity: A A
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- G. Francica, T. J. G. Apollaro, N. Lo Gullo, F. Plastina, "Local Quench, Majorana Zero Modes, and Disturbance Propagation in the Ising chain", **Physical Review B** 94, 245103 (2016).
- A. Molina-Sanchez, M. Palummo, A. Marini, L. Wirtz, "Temperature-dependent excitonic effects in the optical properties of single-layer MoS₂", **Physical Review B** 93(15), 155435 (2016)
- N. Lo Gullo, L. Dell'Anna, "Self-consistent Keldysh approach to quenches in the weakly interacting Bose-Hubbard model", **Physical Review B** 94, 184308 (2016).
- C. Vacacela Gomez, M. Pisarra, M. Gravina, P. Riccardi and A. Sindona, "Plasmon properties and hybridization effects in silicene", **Physical Review B** In Press, 005400 (2017)
- J. Settino, N. Lo Gullo, A. Sindona, J. Goold and F. Plastina, "Signatures of the ground state properties of Tonks-Girardeau and non-interacting Fermi gases in a bichromatic potential", **Physical Review A** in press (2017)
- A. Pedrielli, S. Taioli, G. Garberoglio, N. M. Pugno, "Designing graphene based nanofoams with nonlinear auxetic and anisotropic mechanical properties under tension or compression", **Carbon** 111, 796 (2017)
- L. Matthes, O. Pulci, B. Friedhelm, "Influence of out-of-plane response on optical properties of two-dimensional materials: First principles approach", **Physical Review B** 94(20), 205408 (2016)

INFN Referee Reports (2)

Quality and relevance of the proposed research activity: A A

Project feasibility, including methodology, research plan and strategy: A A

Project impact: A A

Research team qualification and role within the network: A A

Global evaluation: A A

(More to come...)

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Ground State Properties: Kohn-Sham Density Functional Theory

N-Particle
Wave
Function

$$\Psi(1, \dots, N)$$

Many Electrons in the
attractive field of some
structure less atomic Nuclei

Cold Atoms

$$H \Psi = \left[\sum_i^N \frac{-\hbar^2 \nabla_i^2}{2m} + \sum_i^N V_i + \frac{1}{2} \sum_{i \neq j}^N U_{ij} \right] \Psi = E \Psi$$

Stationary
Schrödinger
Equation

$$V_i = \sum_{\alpha} \frac{-Z_{\alpha} e^2}{4\pi\epsilon_0 |\mathbf{r}_i - \mathbf{R}_{\alpha}|} \quad U_{ij} = \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_i - \mathbf{r}_j|}$$

$$V_i \sim V_0 \sin^2(k_0 z_i)$$

$$U_{ij} \sim U_0 \delta(\mathbf{r}_i - \mathbf{r}_j)$$

F. Malet *et al*, PRL 115, 033006 (2015)
A. Sindona *et al*, PRL 111, 165303 (2013)

KS-DFT for Electrons

Variational
Principle

$$\min_{\Psi} \langle \Psi | \hat{H} | \Psi \rangle = E_0 \rightarrow$$

Self-Consistent
KS Equations

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

The ground state properties are
uniquely determined from the
electron density

$$n(\mathbf{r}) = \sum_{i \text{ occ}} |\psi_i(\mathbf{r})|^2$$

Independent quasi
(KS) electrons

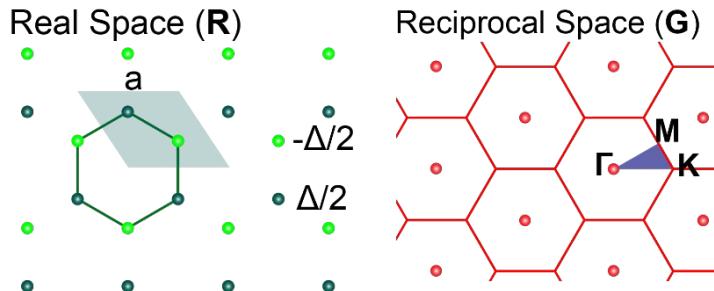
Electron-Nuclear
Interaction

$$V_{KS} = V_{ext}(\mathbf{r}) + \int d^3 r' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \frac{\delta E_{xc}}{\delta n(\mathbf{r})}$$

Exchange and
Correlation (LDA,GGA)

KS-DFT Packages Available in Galileo and Marconi

Periodic Systems



$a=2.46 \text{ \AA}$ $\Delta=0$ (Graphene)

$a=3.82 \text{ \AA}$ $\Delta=0.45 \text{ \AA}$ (Silicene)

$a=4.00 \text{ \AA}$ $\Delta=0.86 \text{ \AA}$
(Germanene)

Plane-Wave DFT

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

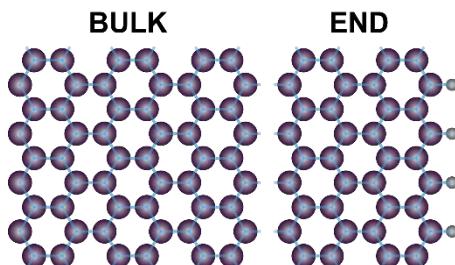
abinit/7.10.5
espresso++/1.9.2
vasp/5.4.1

Localized Orbital DFT

$$\psi_{\nu k}(\mathbf{r}) = \sum_{\mathbf{R}} c_{\nu \mathbf{R}} \varphi_{\nu}(\mathbf{r} - \mathbf{R}) e^{i \mathbf{k} \cdot \mathbf{R}}$$

siesta/4.1-b2
crystal14/1.0.4

Clusters



Typical runs: $\sim 10^3$ atoms
Limit $\sim 30,000$ atoms

Gaussian Type Orbital DFT

$$\psi_i(\mathbf{r}) = \sum_b c_{ib} g_b(\mathbf{r})$$

gamess/5dic2015
nwchem/6.6
gaussian16/A.03

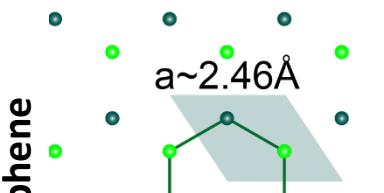
$$\psi_{v\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} \frac{c_{v\mathbf{k}+\mathbf{G}}}{\sqrt{\Omega}} e^{i(\mathbf{k}+\mathbf{G}) \cdot \mathbf{r}}$$

v band index
k wave vector in IrrBZ

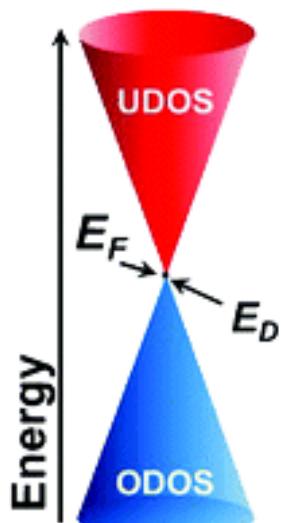
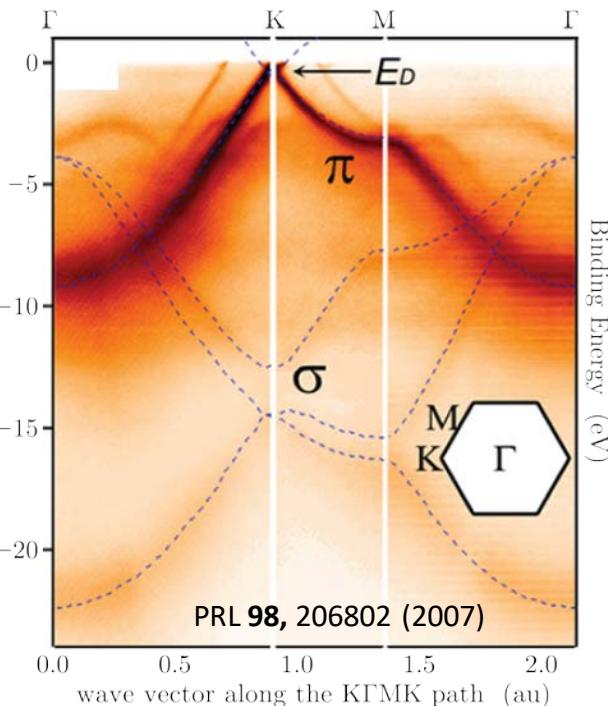
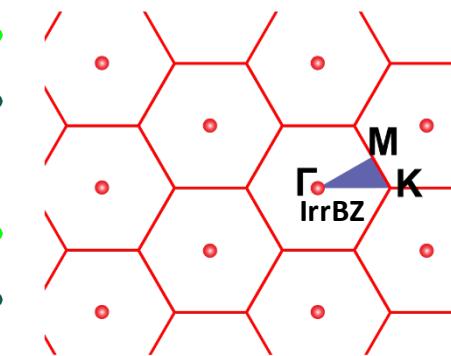
$$\varepsilon_{v\mathbf{k}}$$

Real Space (R)

Graphene



Reciprocal Space (G)



Geometry
Optimization
(SC Run)
<50 Coreh

Ground State
Density
(SC Run)
<10 Coreh

Ground State
Wave functions
(Non SC Run)
 10^2 - 10^3 Coreh

~5000 coefficients $c_{v\mathbf{k}+\mathbf{G}}$ per wavefunction $\psi_{v\mathbf{k}}$
~50000 k-points in the IrrBZ
~10-60 bands
Output file ~ 50 Gb

Modules....

intel/cs-xe-2015--binary
intelmpi/5.0.3--binary
mkl/11.3.0--binary
hdf5/1.8.14_ser-intel--cs-xe-2015--binary
netcdf/4.1.3--intel--cs-xe-2015--binary
abinit/7.10.5

Electron Density

$$n(\mathbf{r}) = \sum_{v\mathbf{k} \in \text{IrrBZ}}^{occ} w_{\mathbf{k}} |\psi_{v\mathbf{k}}(\mathbf{r})|^2$$

PW-DFT

KS-Electron WFs

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

v band index
k wave vector in IrrBZ

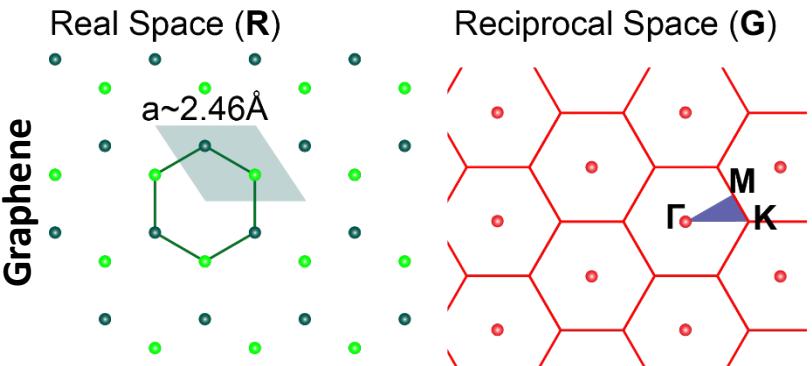
Band Energies

$$\epsilon_{vk}$$



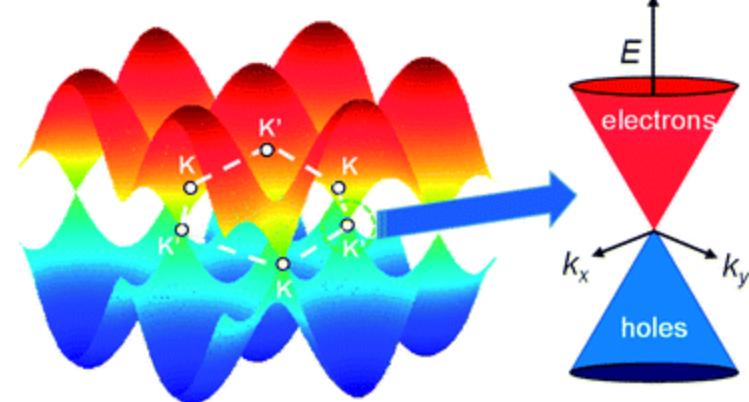
Real Space (**R**)

Graphene



Reciprocal Space (**G**)

Massless
Dirac Fermions



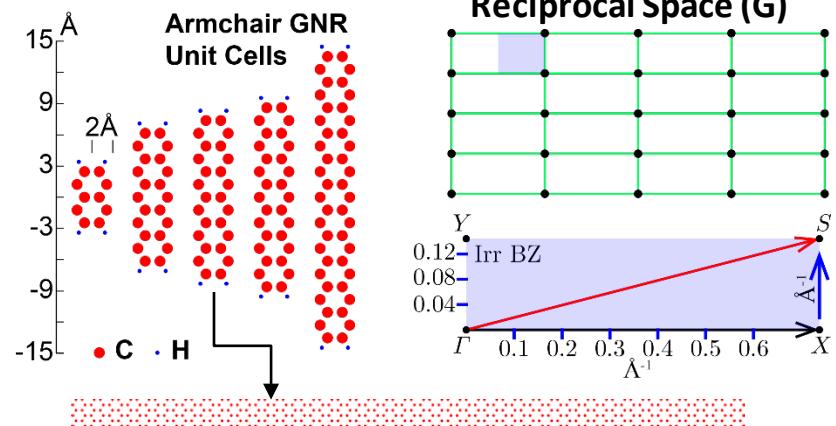
Graphene Nanoribbons

Reciprocal Space (**G**)

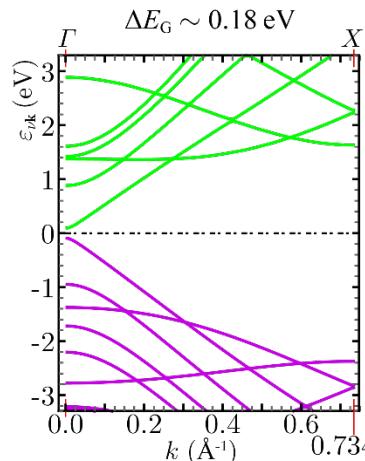
Geometry
Optimization
(SC Run)
 $\sim 10^3$ Coreh

Ground State
Density
(SC Run)
 $\sim 10^2$ Coreh

Ground State
Wave functions
(Non SC Run)
 $\sim 10^3$ Coreh



Real Space (**R**)



~10⁵ coefficients $c_{v\mathbf{k}+\mathbf{G}}$ per wavefunction ψ_{vk}
~10000 k-points in the IrrBZ
~10-60 bands
Output file ~ 100 Gb

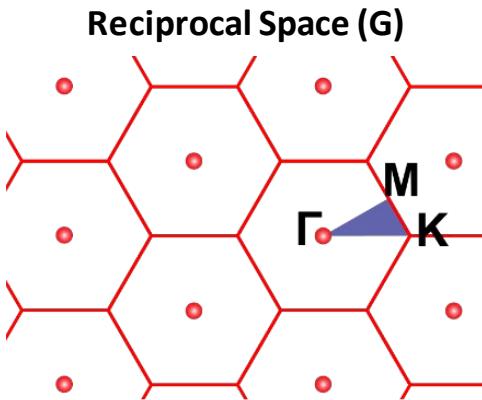
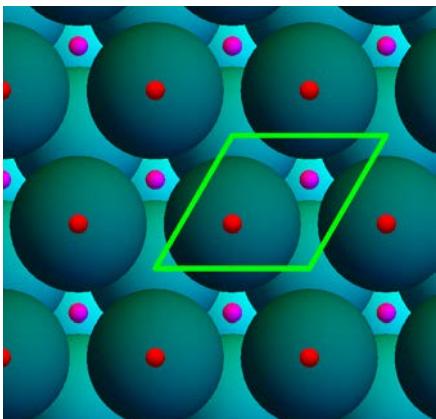
C. Vacacela Gomez, M. Pisarra, M. Gravina, J. M. Pitarke, and A. Sindona, *Phys. Rev. Lett.* **117**, 116801 (2016)
C. Vacacela Gomez, M. Pisarra, M. Gravina, and A. Sindona, *Beilstein J. Nanotechnol.* **2017**, *8*, 172 (2017)

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

v band index
k wave vector in IrrBZ

$$\varepsilon_{\nu k}$$

Graphene on (Nickel or Copper)



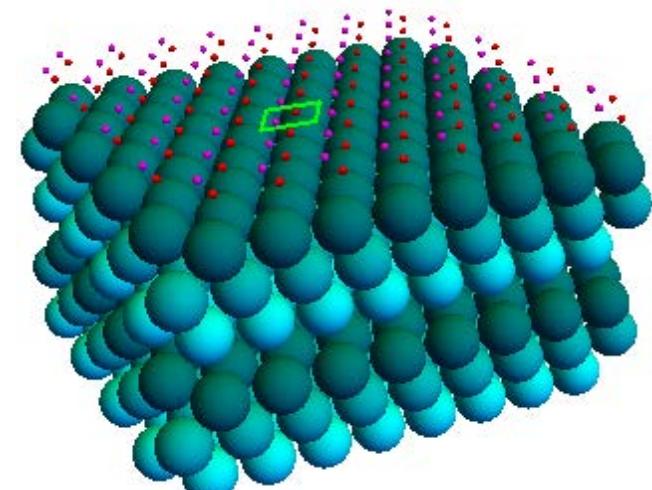
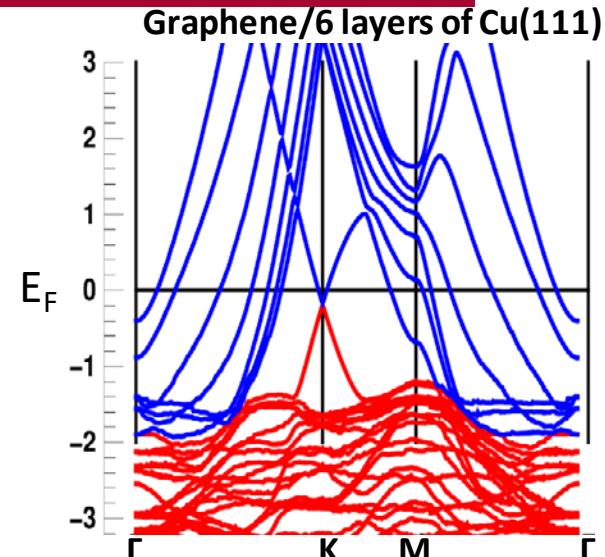
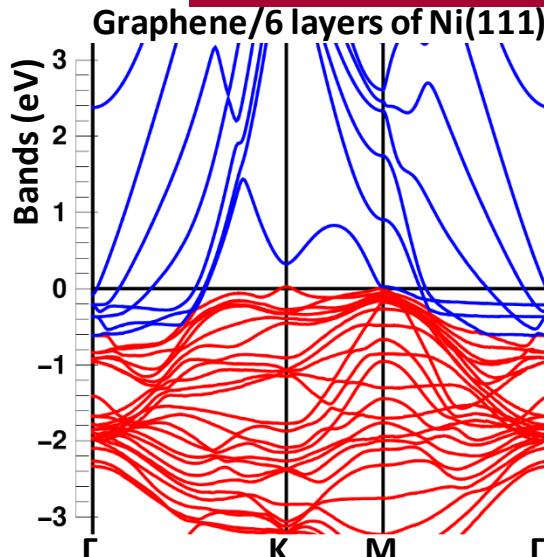
Geometry
Optimization
(SC Run)
 $\sim 10^3$ Coreh

Ground State
Density
(SC Run)
 $\sim 10^3$ Coreh

Ground State
Wave functions
(Non SC Run)
 $\sim 10^4$ Coreh

$\sim 10^4$ coefficients $c_{\nu k + G}$ per wavefunction $\psi_{\nu k}$
 $\sim 10^4\text{-}10^5$ k-points in the IrrBZ
 $\sim 50\text{-}100$ bands
Output file ~ 100 Gb

Presence/Absence of Massless Dirac Fermions



PW-DFT >10kCoreh

KS-Electron WFs

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

Band Energies

$$\varepsilon_{\nu k}$$



The NEMESYS Project
UNICAL-LNF-ToV-TIFFPA

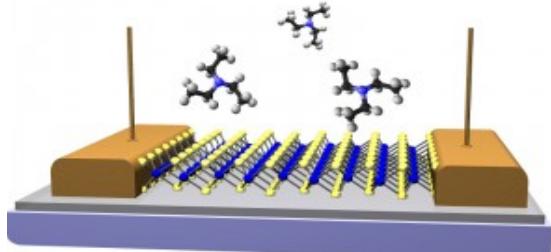
Transition Metal Dichalcogenides (TMDC): novel 2D materials beyond graphene

H	MX ₂ M = Transition-metal X = Chalcogen												He					
	Li	Be																
Na	Mg	3	4	5	6	7	8	9	10	11	12							
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	S	Cl	Ne	Ar
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	Br	Kr	
Cs	Ba	La-Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	I	Xe	
Fr	Ra	Ac-Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo	

Semiconductors - Insulators - Metals and
Topological Insulators!!

Gas sensors

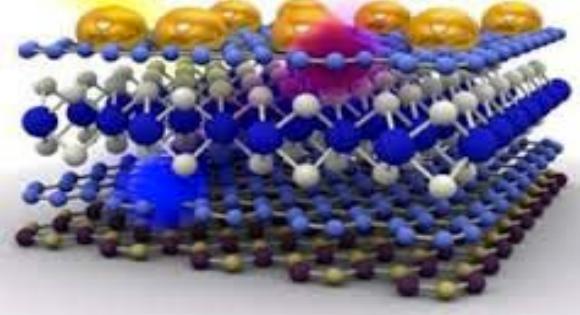
Perkins et al Nanoletter 2013



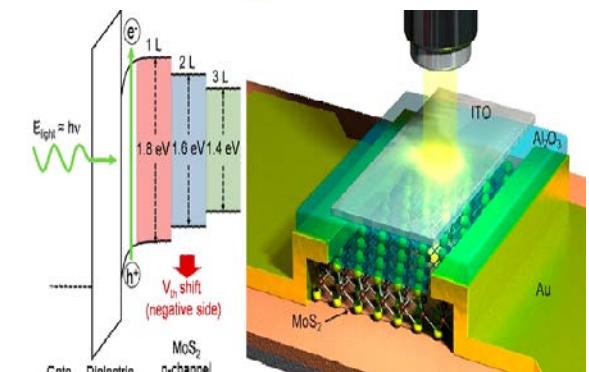
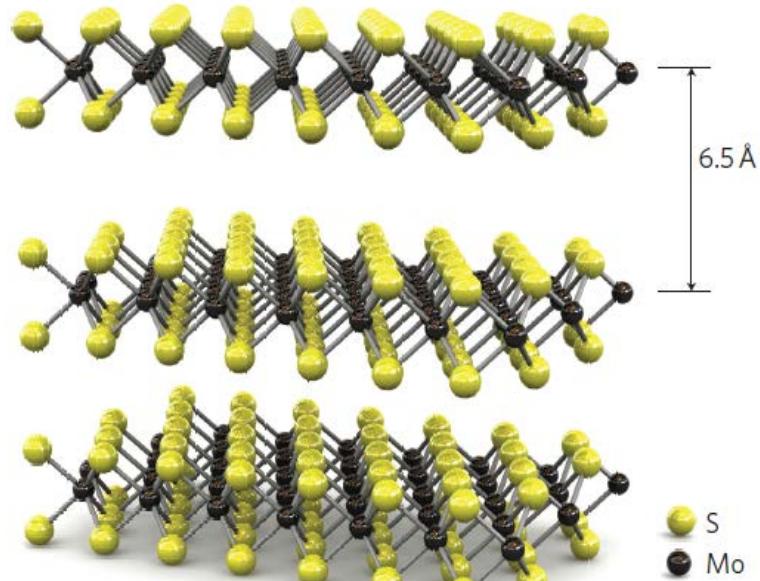
PV solar cells

Britnell et al Science 2013

Bernardi Palummo Grossman NL 2013



Molybdenum disulfide



Top-gate modulated Photo-transistor
H.S .Lee et al. Nano Lett. 2012, 12, 3695

PW-DFT

Eigenvectors

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

v band index
k wave vector in IrrBZ

Eigenvalues $\varepsilon_{\nu k}$

Self-Consistent KS Potential

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

Electron Density

$$n(\mathbf{r}) = \sum_{\nu k \in \text{IrrBZ}}^{\text{occ}} w_k |\psi_{\nu k}(\mathbf{r})|^2$$

Linear Response Theory

Small perturbation

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

Unperturbed density-density response

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

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

$$\chi_{GG'}^{\pm 0}(\omega, \mathbf{q}) = \frac{2}{\Omega} \sum_{\mathbf{k}} \sum_{\nu, \nu'} \frac{\left(f_{\varepsilon_{\nu k}} - f_{\varepsilon_{\nu' k+q}} \right) \rho_{\nu \nu'}^{\mathbf{k} \mathbf{q}}(\mathbf{G}) \rho_{\nu \nu'}^{\mathbf{k} \mathbf{q}}(\mathbf{G}')^*}{\hbar \omega + \varepsilon_{\nu k} - \varepsilon_{\nu' k+q} \pm i\eta}$$

$$\rho_{\nu \nu'}^{\mathbf{k} \mathbf{q}}(\mathbf{G}) = \sum_{\mathbf{G}'} c_{\nu \mathbf{k} + \mathbf{G}'}^* c_{\nu' \mathbf{k} + \mathbf{q} + \mathbf{G} + \mathbf{G}'}^*$$

$$\text{Full Polarizability } \chi_{GG'} = \chi_{GG'}^0 + (\chi_0 \nu \chi)_{GG'} = [\chi_0 (1 - \nu \chi_0)^{-1}]_{GG'}$$

Screening
(Plasmon Properties)

$$(\epsilon^{-1})_{GG'} = \epsilon_0 (1 + \nu \chi)_{GG'} \approx \epsilon_0 [(1 - \nu \chi_0)^{-1}]_{GG'}$$

Dynamically
screened
interaction

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

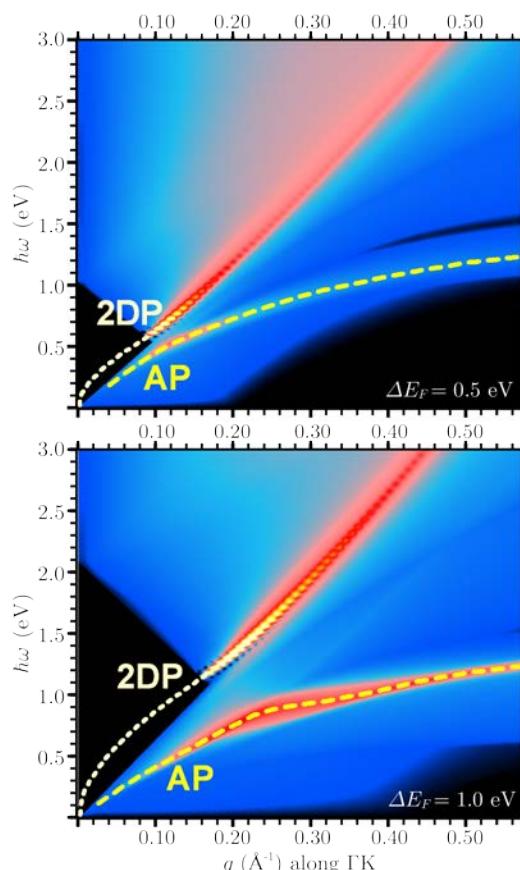
Macroscopic Average

$$\text{Re}[\epsilon_{\alpha\alpha}(q, \nu)] = 0$$

$$\text{Im}[\epsilon_{\alpha\alpha}(q, \nu)]$$

$$-\text{Im}[\epsilon_{\alpha\alpha}(q, \nu)^{-1}]$$

Graphene



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

Plasmon Resonances

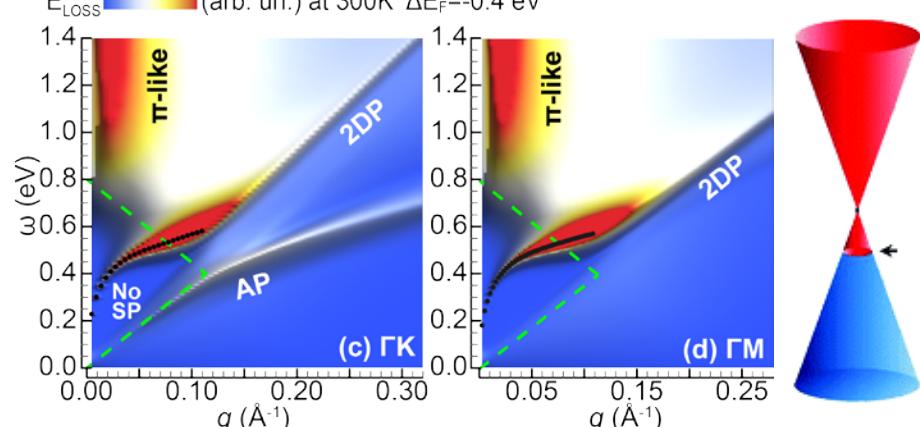
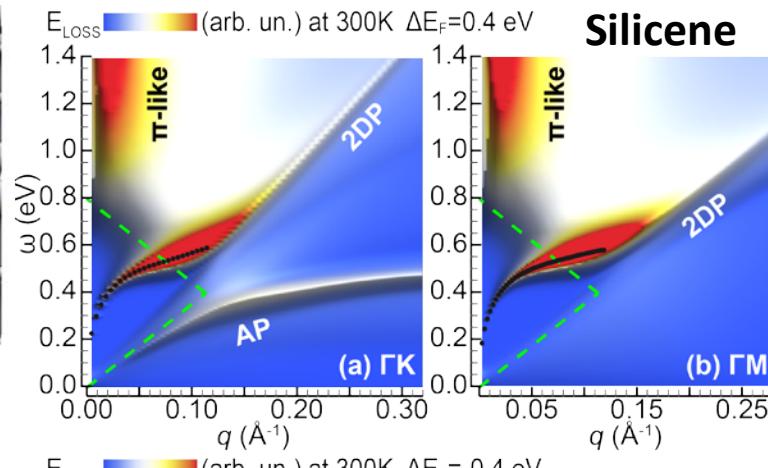
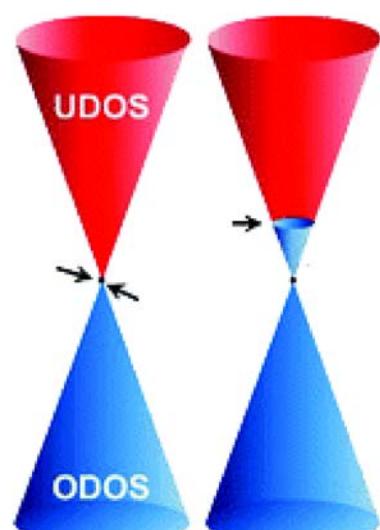
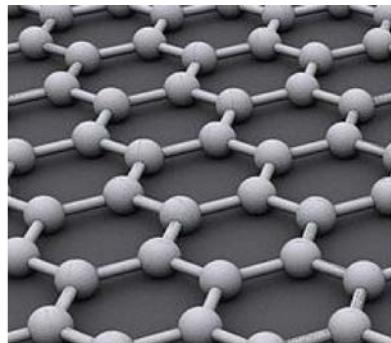
Absorption Spectrum

**Loss Function
(Plasmon Spectrum)**



~100 Coreh per q point!!!

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)



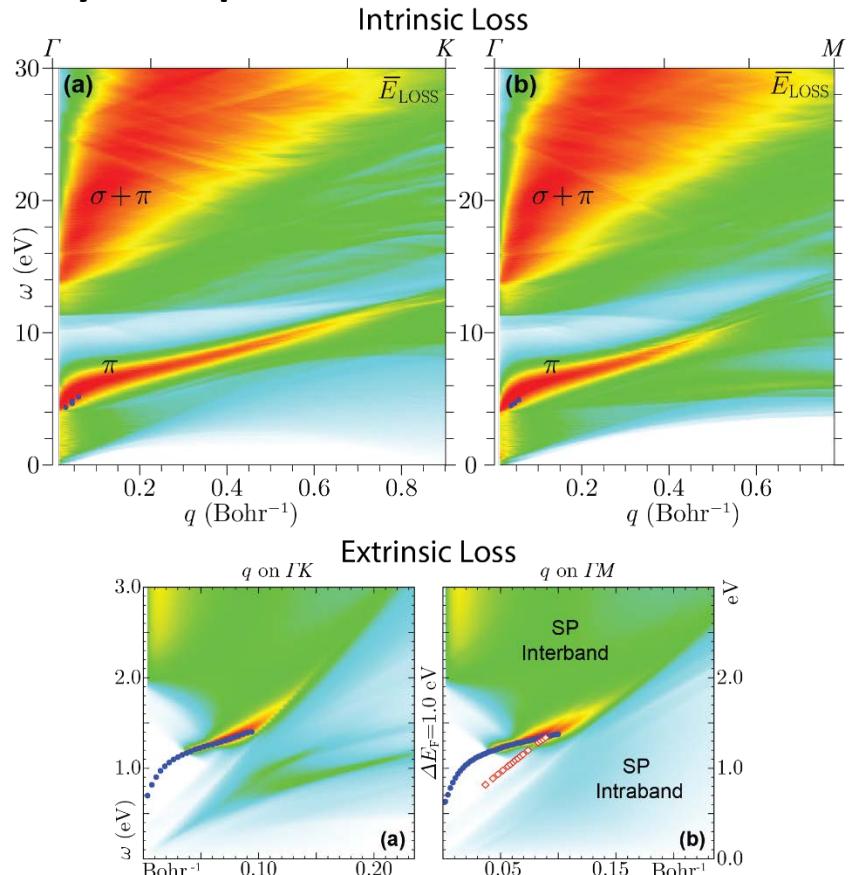
Macroscopic Average

$$\text{Re}[\epsilon_{\alpha\alpha}(q, \nu)] = 0$$

$$\text{Im}[\epsilon_{\alpha\alpha}(q, \nu)]$$

$$-\text{Im}[\epsilon_{\alpha\alpha}(q, \nu)^{-1}]$$

Bilayer Graphene



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

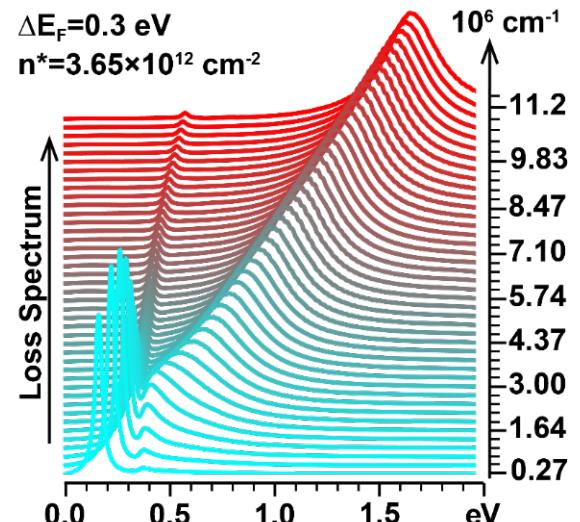
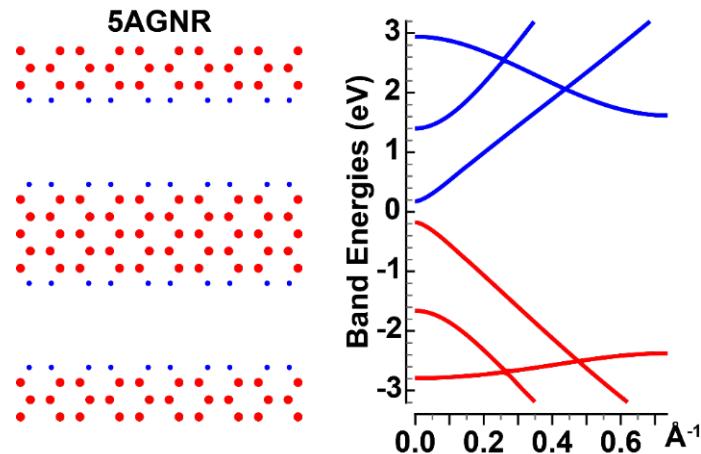
Plasmon Resonances

Absorption Spectrum

Loss Function
(Plasmon Spectrum)

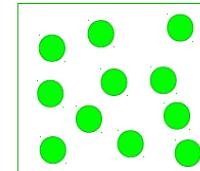
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M. Pisarra, A. Sindona, P. Riccardi, V. M. Silkin, J. M. Pitarke, **New Journal of Physics** 16, 083003 (2014); M. Pisarra, A. Sindona, M. Gravina, V. M. Silkin, J. M. Pitarke, **Physical Review B** 93, 035440 (2016); C. Vacacela Gomez, M. Pisarra, 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** 96, 005400 (2017)



Self-Consistent KS Potential

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



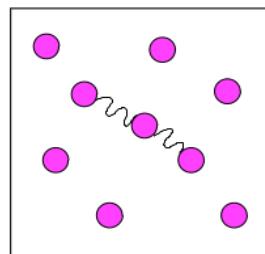
$$\psi_{v\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} \frac{c_{v\mathbf{k}+\mathbf{G}}}{\sqrt{\Omega}} e^{i(\mathbf{k}+\mathbf{G}) \cdot \mathbf{r}} \quad \left[\frac{-\hbar^2 \nabla^2}{2m} + V_{KS} \right] \psi_{v\mathbf{k}} = \varepsilon_{v\mathbf{k}} \psi_{v\mathbf{k}}$$

Ground State Properties: Poor predictions for electronic band gaps!!

GW

$$\left[\frac{-\hbar^2 \nabla^2}{2m} + V_{ext}(\mathbf{r}) + V_H(\mathbf{r}) + \int d^3 r' \Sigma(\mathbf{r}, \mathbf{r}', \varepsilon'_{v\mathbf{k}}) \right] \psi'_{v\mathbf{k}} = \varepsilon'_{v\mathbf{k}} \psi'_{v\mathbf{k}}$$

$\psi_{v\mathbf{k}}$ $\varepsilon_{v\mathbf{k}}$



Weakly interacting
quasi-particles
(QP equation)

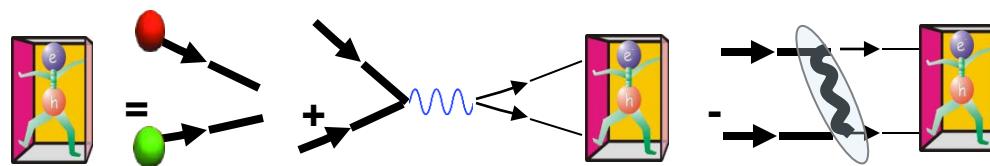
Charged electronic
excitations (bands,
bandoffsets ..)

χ^0
RPA polarisability

$\Sigma = iGW$
GW self-energy
correction
calculated

BSE

$\epsilon = 1 - v\chi^0$
 ϵ^{-1}



Propagation of Interacting e-h couples

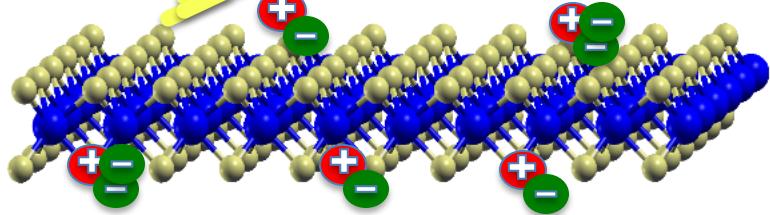
INCREASING COMPUTATIONAL COST

Transition Metal Dichalcogenides

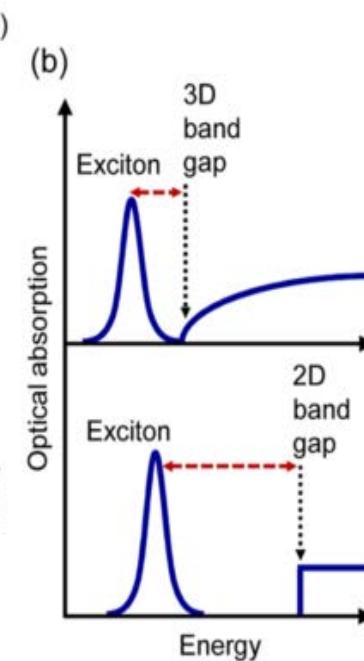
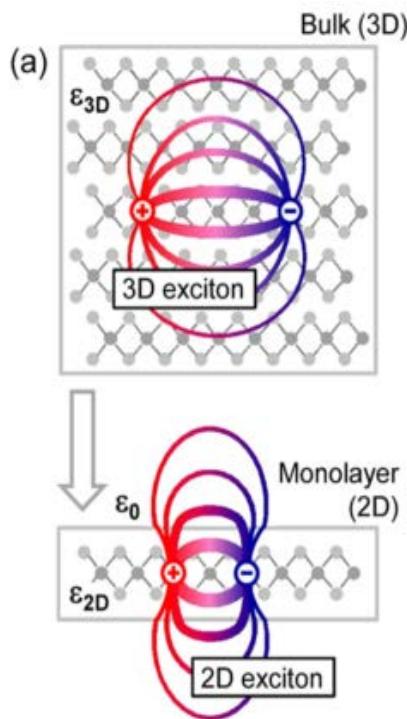
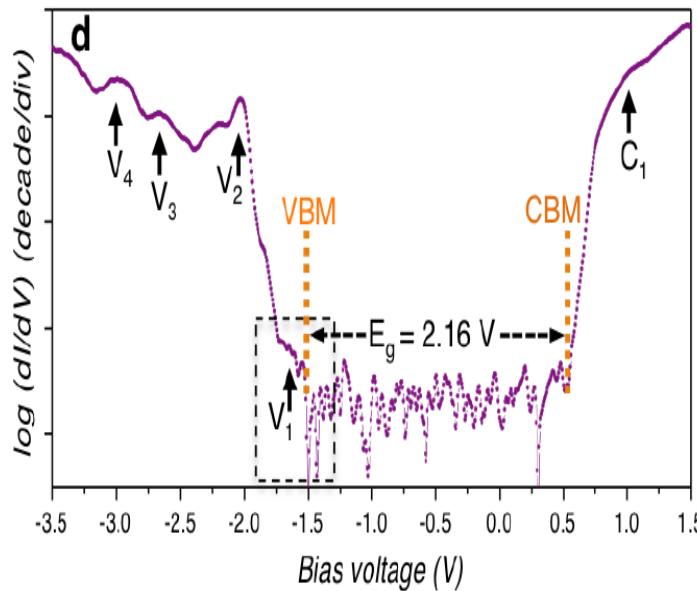
Excitons

Trions

Biexcitons

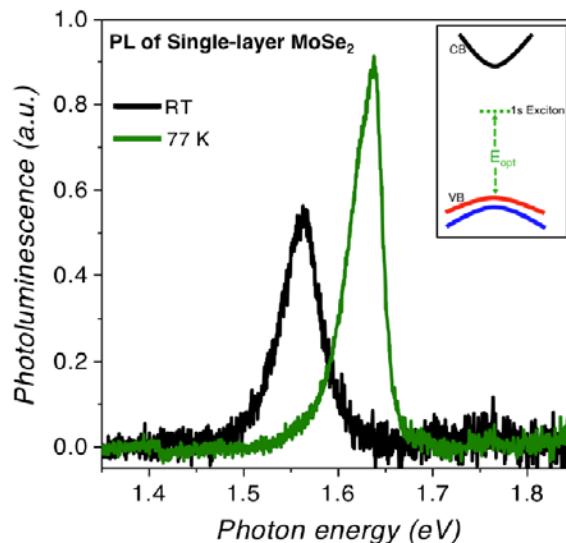


A. Chernikov et al PRL 113 (2014)



Low dimensional screening: enhanced e-e (e-h) interaction

Many-body effects dominate the opto-electronic properties



PL peak due to Strongly bound exciton

b.e. = 0.55 eV for MoSe2 on Bilayer graphene

Ugeda et al. Nature Mat. (2014)

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

Y. Pavlyukh, A. M. Uimonen, G. Stefanucci, R. van Leeuwen, "Vertex Corrections for Positive-Definite Spectral Functions of Simple Metals", **Physical Review Letters** 117, 206402 (2016)

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)

A. Michele, K. Thanayut, A. Zobelli, M. Palummo, R. Rurali, "Crystal Phase Effects in Si Nanowire Polytypes and Their Homojunctions", **Nano Letters** 16, 5694 (2016)

G. Francica, J. Goold, M. Paternostro, F. Plastina, "Daemonic Ergotropy: Enhanced Work Extraction from Quantum Correlations", **Nature Quantum Information** in Press (2017).

A. Sindona, "Orthogonality Catastrophe and Decoherence in a Trapped-Fermion Environment", **Physical Review Letters** 111, 165303 (2013)