Electronic and optical properties of nano-materials

Claudio Attaccalite

CNRS concours 03/01 (2023)

Short CV

2001: Master in Physics, La Sapienza University (Rome)

2005: PhD in Physics, SISSA, Trieste (Italie) *S. Sorella*

2006-2007: PostDoc, IEMN, Lille, *L. Wirtz*

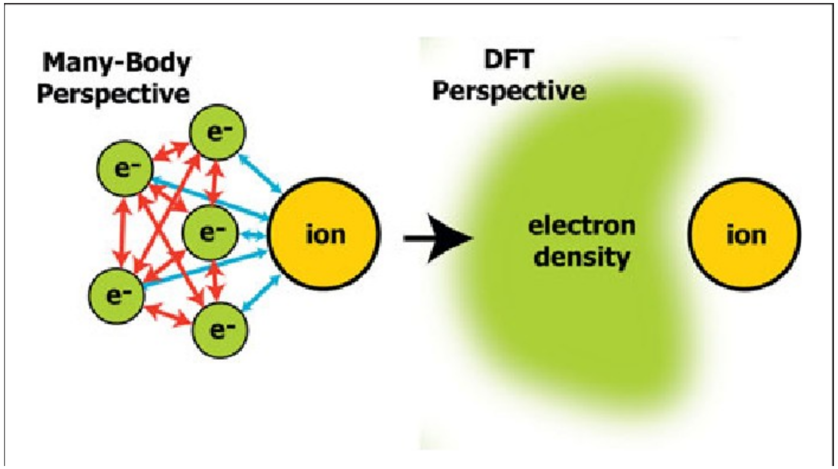
2008-2009: PostDoc, Universidad del Pais Vasco, *A. Rubio*

2009-2014: CNRS Researcher (CR2), Institute Néel, France

2014- : CNRS Researcher (CR1), CINaM, France

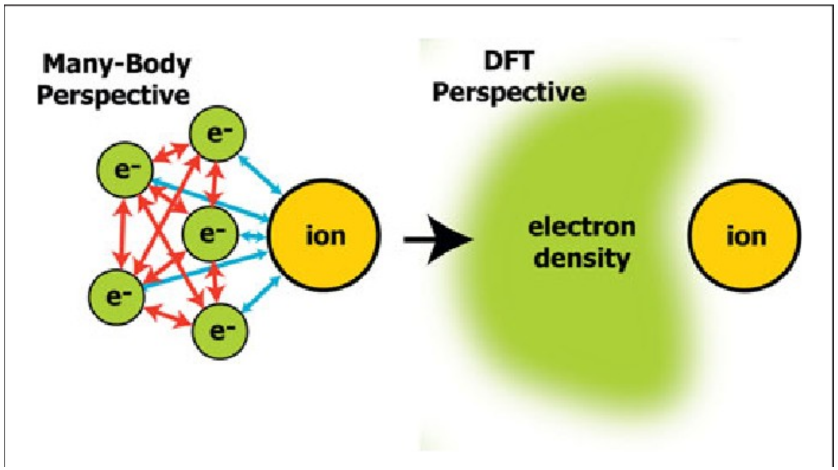
2018-2019: Visiting Researcher, Tor-Vergata Univ. (Rome)

My philosophy 1/2



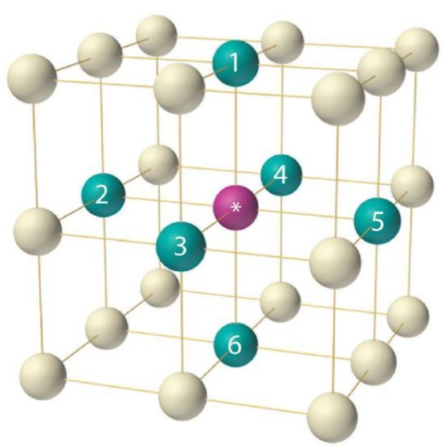
Density Functional Theory

My philosophy 1/2

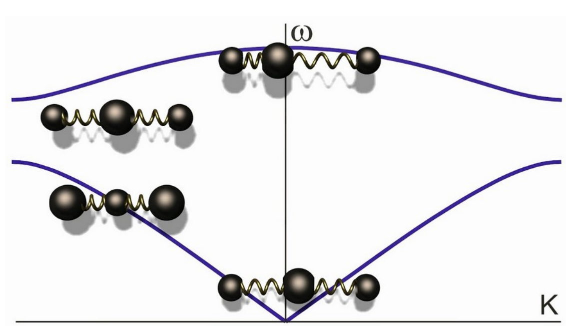


Density Functional Theory

Atomic structure

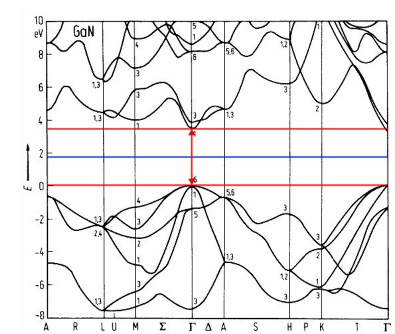


Vibrational properties



A starting Hamiltonian

$$H_0 = T + V_{ion} + V_{ks}(\rho_0)$$

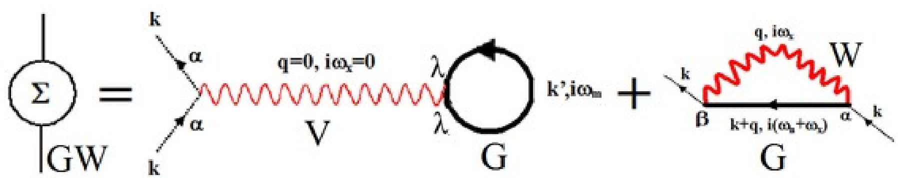


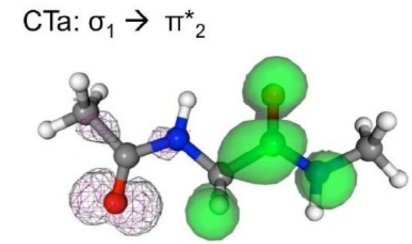
My philosophy 2/2

Green's function theory

Quasi-particles

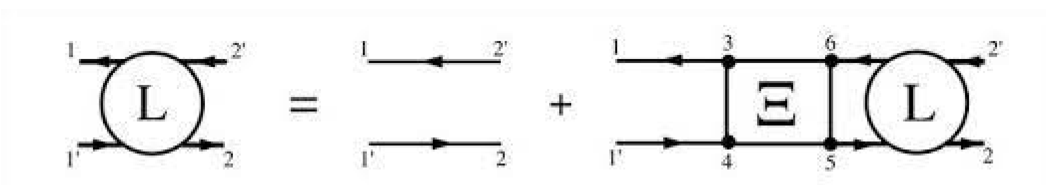
$$G = G_0 + G_0 \Sigma G$$

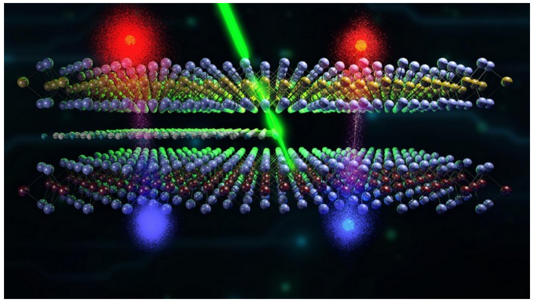




Excited states

Linear response



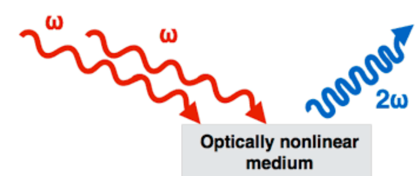


Optical properties

Real-time dynamics

$$-i \frac{\partial \psi(t)}{\partial t} = H_{eff} \psi(t)$$

$$P(\omega) = P_0 + \chi^{(1)} E + \chi^{(2)} E^2 + O(E^3)$$



Non-linear response

Code development

Yambo

Siesta!

TurboRVB
Quantum Monte Carlo Package SISSA

D. Sangalli, A. Ferretti, H. Miranda, **C. Attaccalite,** et al. J. Phys. Cond. Matt. 31, 325902 (2020)
K. Nakano, **C. Attaccalite** et al. J. Chem. Phys. 152, 204121 (2020)

Code development

D. Sangalli, A. Ferretti, H. Miranda, **C. Attaccalite,** et al. J. Phys. Cond. Matt. 31, 325902 (2020)
K. Nakano, **C. Attaccalite** et al. J. Chem. Phys. 152, 204121 (2020)

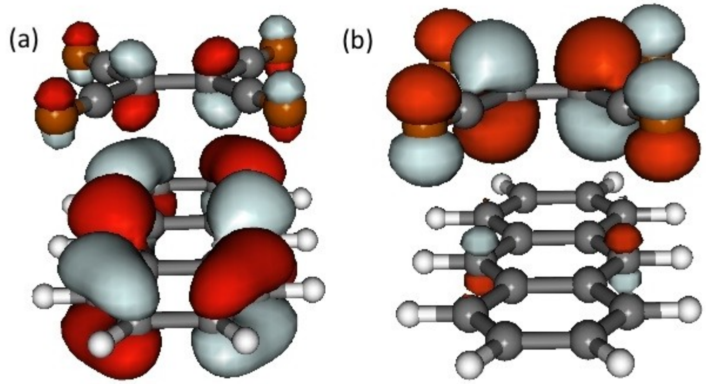
Code development

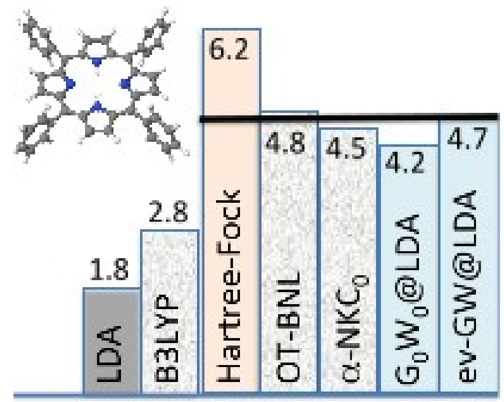
Users interaction

Yambo **school** 2022
40 participants

D. Sangalli, A. Ferretti, H. Miranda, **C. Attaccalite,** et al. J. Phys. Cond. Matt. 31, 325902 (2020)
K. Nakano, **C. Attaccalite** et al. J. Chem. Phys. 152, 204121 (2020)

Excited states in molecules

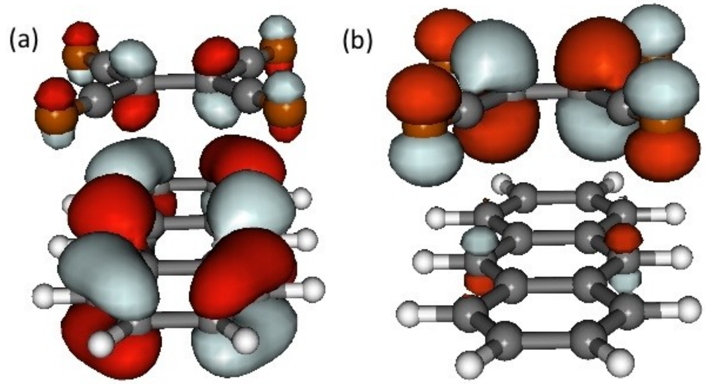


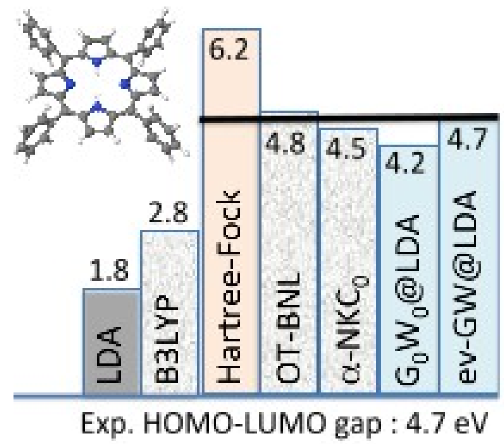


X. Blase and **C. Attaccalite** Appl. Phys. Lett. 99, 171909 (2011)

X. Blase, **C. Attaccalite**, and V. Olevano Phys. Rev. B 83, 115103 (2011)

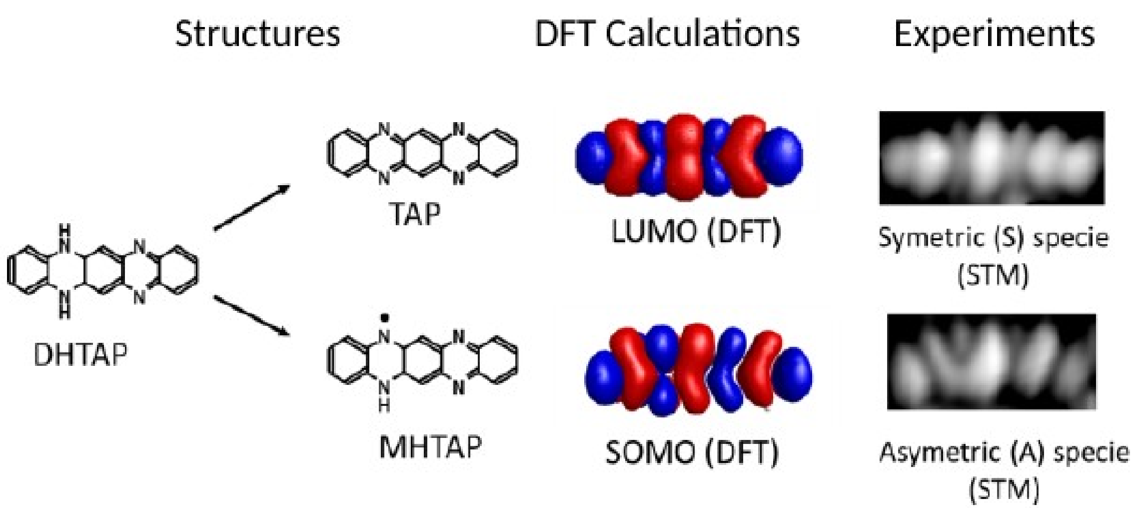
Excited states in molecules

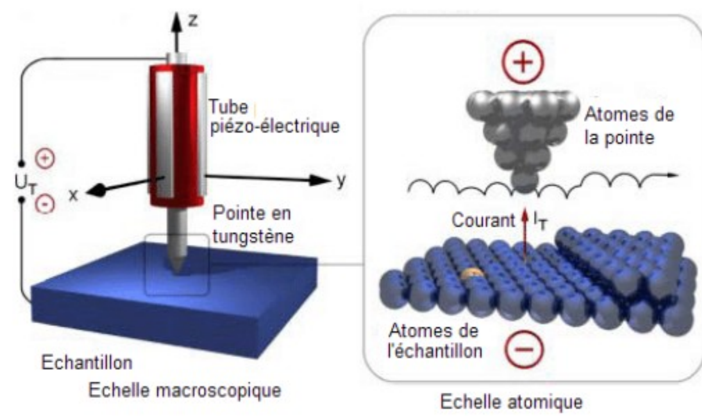




X. Blase and **C. Attaccalite** Appl. Phys. Lett. 99, 171909 (2011)
X. Blase, **C. Attaccalite**, and V. Olevano Phys. Rev. B 83, 115103 (2011)

Molecules on surfaces



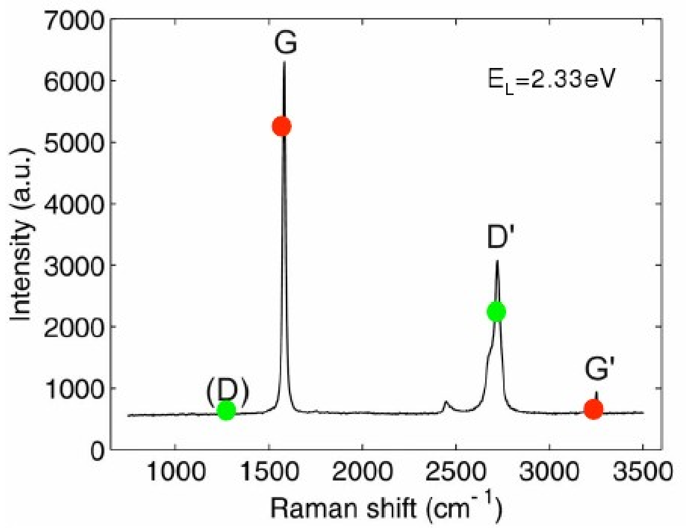


A. D'Aléo, A. Saul, **C. Attaccalite** and F. Fages, Mater. Chem. Front, 3, 86-92 (2019)
T. Leoni, T. Lelaidier, A. Thomas, A. Ranguis, O. Siri, **C. Attaccalite** et al. Nanoscale (2023)

Electron phonon coupling

Correlation effects in the EPC

RAMAN



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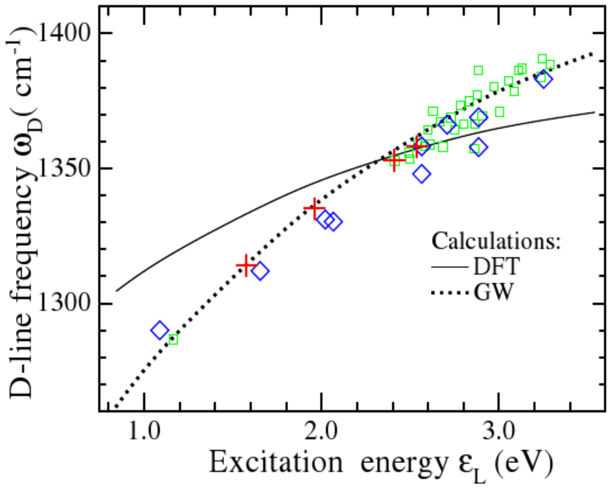

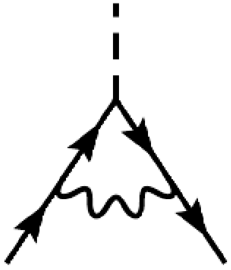

Electron phonon coupling

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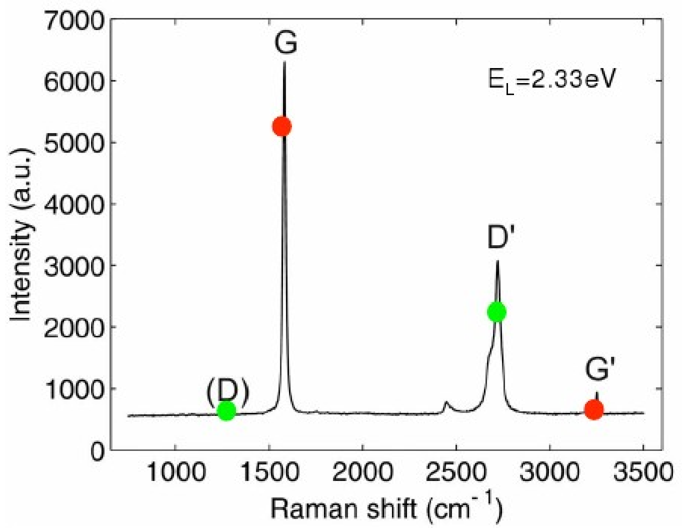
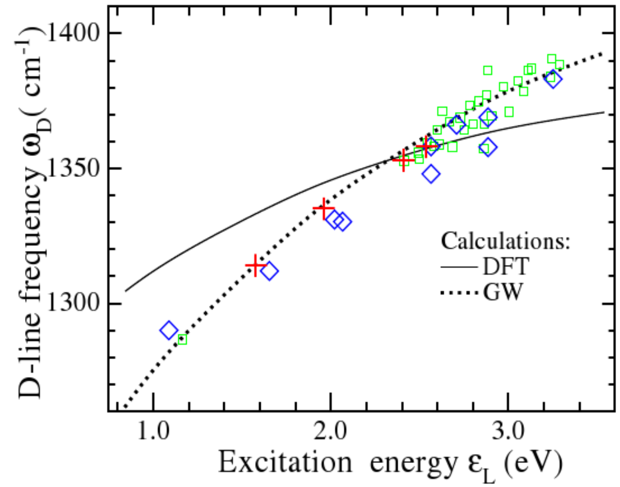
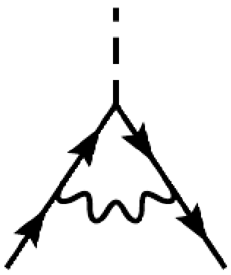
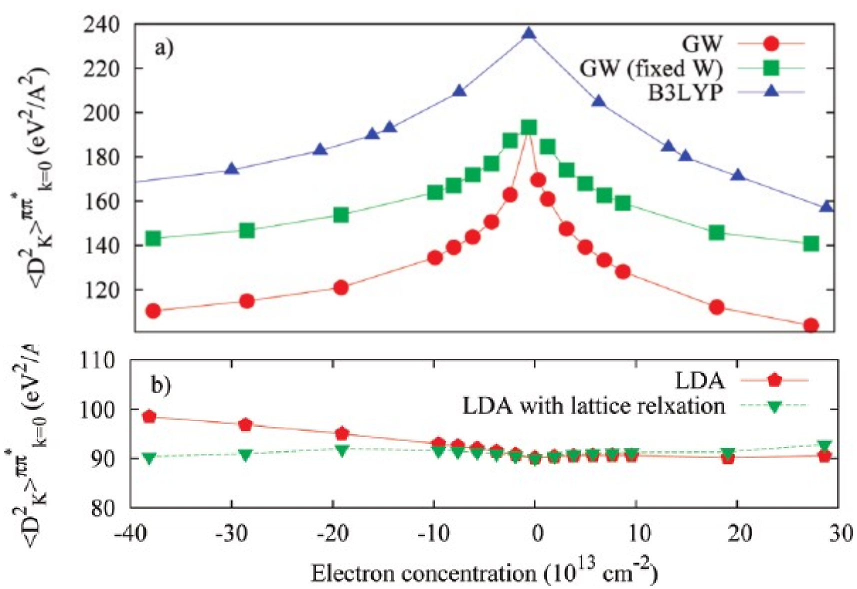


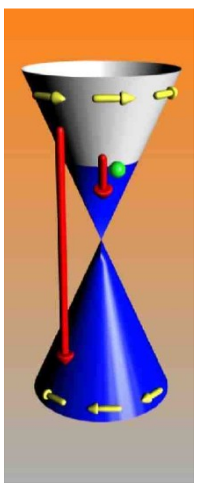
RAMAN

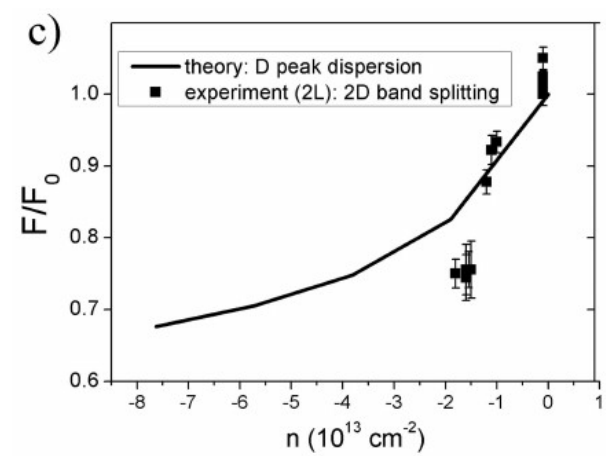




Doping effect





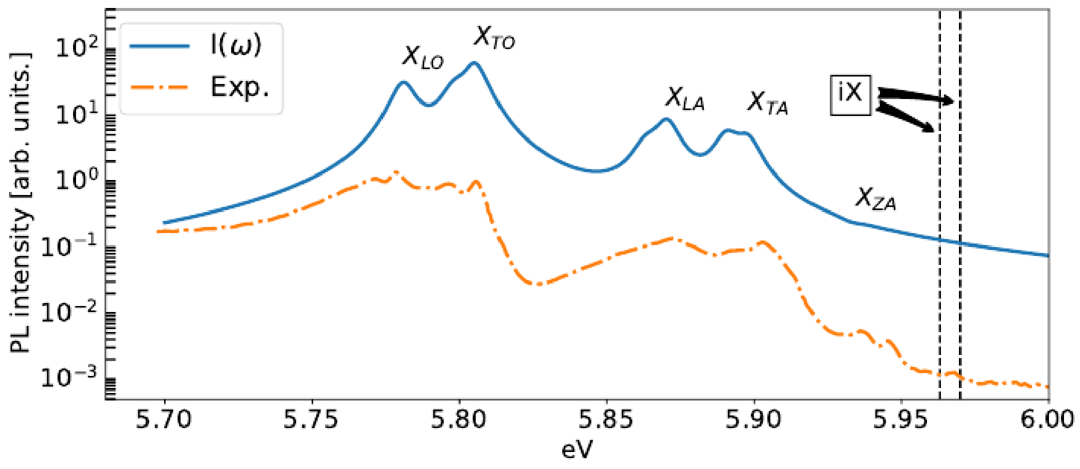


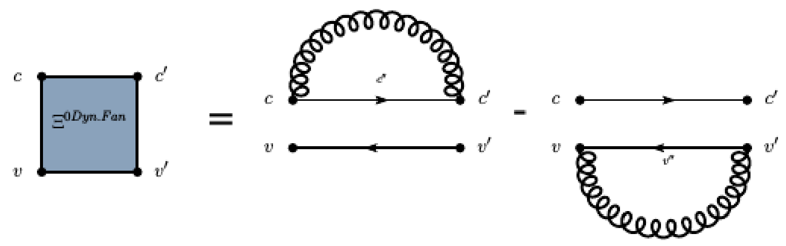
Matteo Bruna and Stefano Borini
Phys. Rev. B **83**, 241401(R) (2011)

C. Attaccalite et al., Nanoletters, **10**, 1172(2010)

Exciton phonon coupling (finite differences)

Phonon-induced luminescence

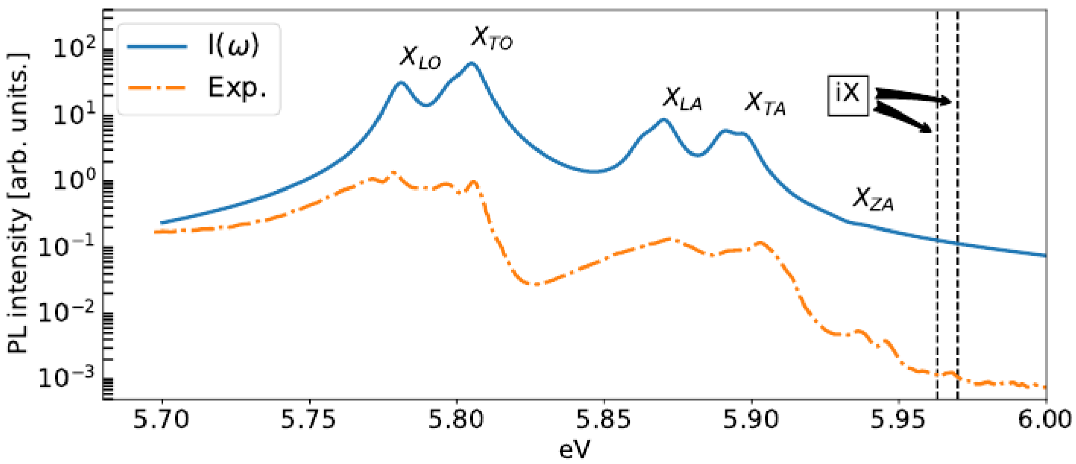


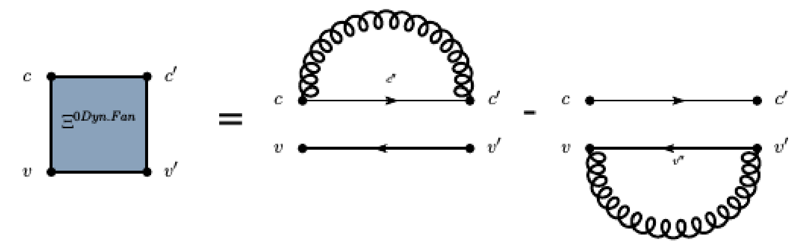


E. Cannuccia, B. Monserrat, **C. Attaccalite,** PRB B 99, 125403 (2019)

Exciton phonon coupling (finite differences)

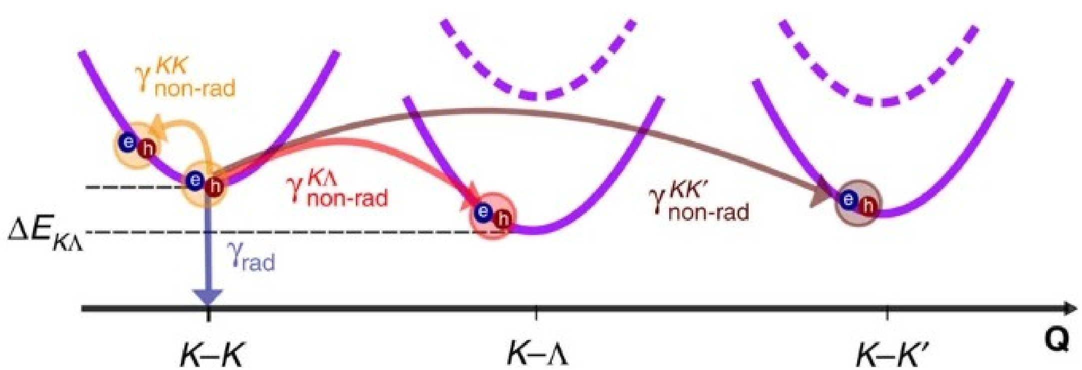
Phonon-induced luminescence

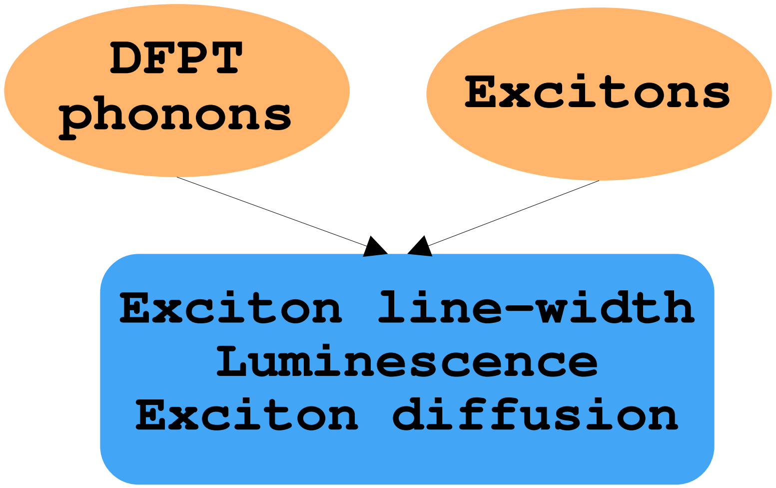




E. Cannuccia, B. Monserrat, **C. Attaccalite,** PRB B 99, 125403 (2019)

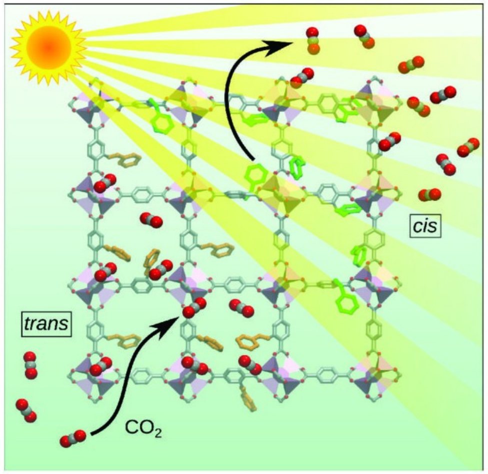
Exciton-phonon coupling from first principles



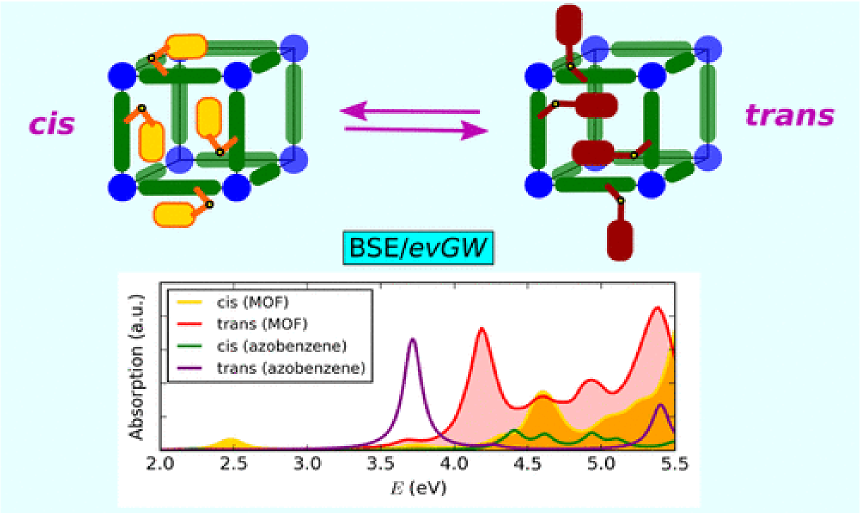


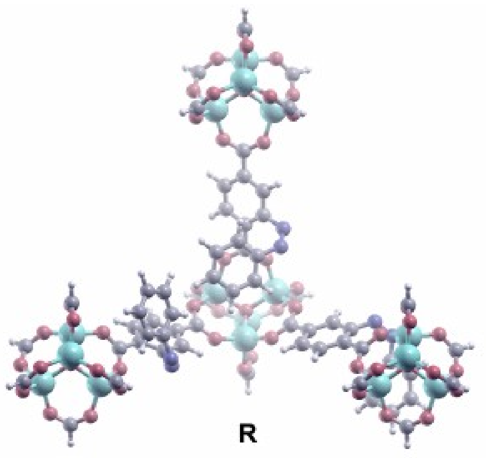
P. Lechifflart, F. Paleari, D. Sangalli, **C. Attaccalite,** PRM 7, 024006 (2023)

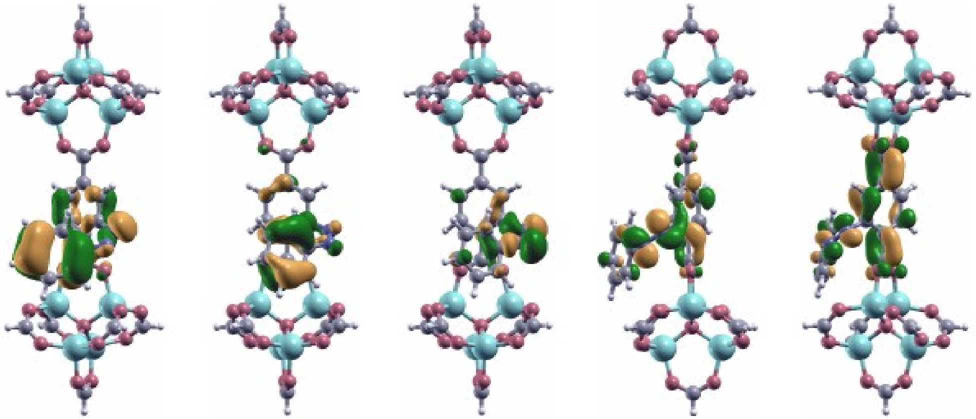
Metal organic frameworks (MOF)



Collaboration with SIMAP (Grenoble)
financed by ANR

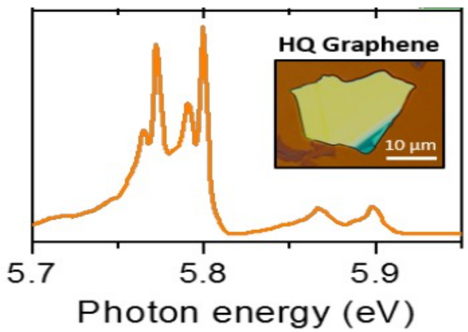






A. R. Kshirsagar, **C. Attaccalite**, X. Blase, J. Li, and R. Poloni, J. of Phys. Chem. C **125**, 7401(2021)
A. R. Kshirsagar, X. Blase, **C. Attaccalite**, R. Poloni . J. Phys. Chem. Lett. , **12**, 4045 (2021)

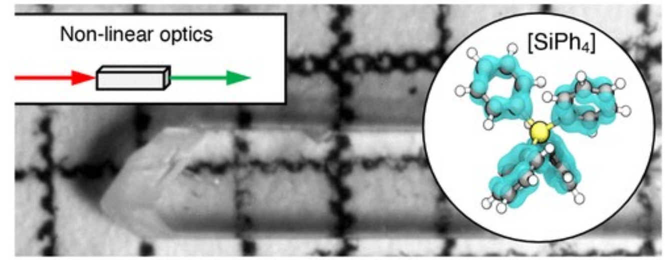
Internal / External collaborations



EELS and luminescence
A.Loiseau, J.Barjon (2017-)

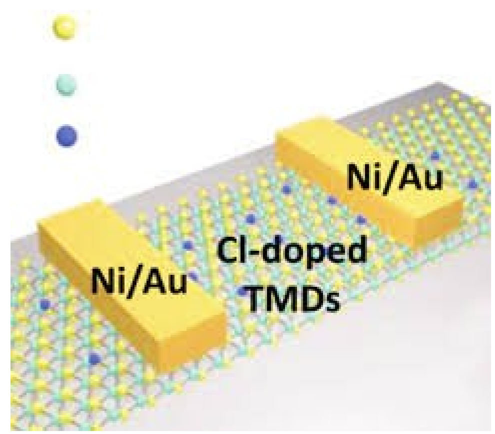
ONERA
THE FRENCH AEROSPACE LAB

Graphene Flagship



Invited Prof. at UNIVERSITÄT PADERBORN

New non-linear crystals
S.Sanna, S.Chatterjee (2020-)

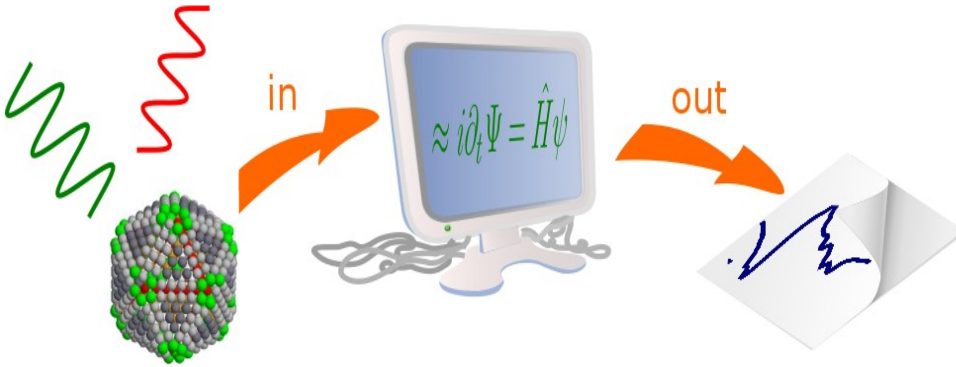


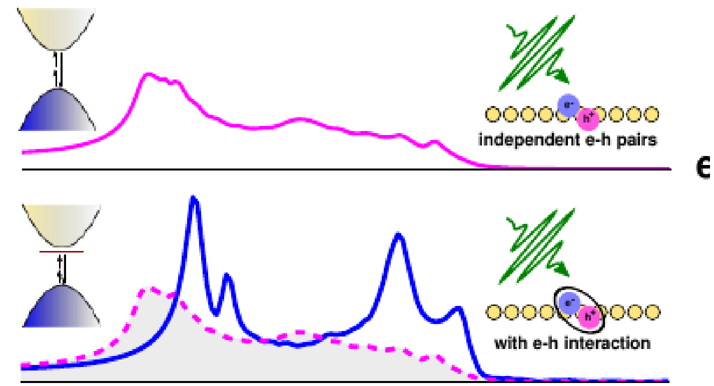
PhD thesis AGENCE NATIONALE DE LA RECHERCHE ANR

Opto-electronics with 2D materials
R.Parret (2021-)

Non-linear spectroscopy

Second and third harmonic generation

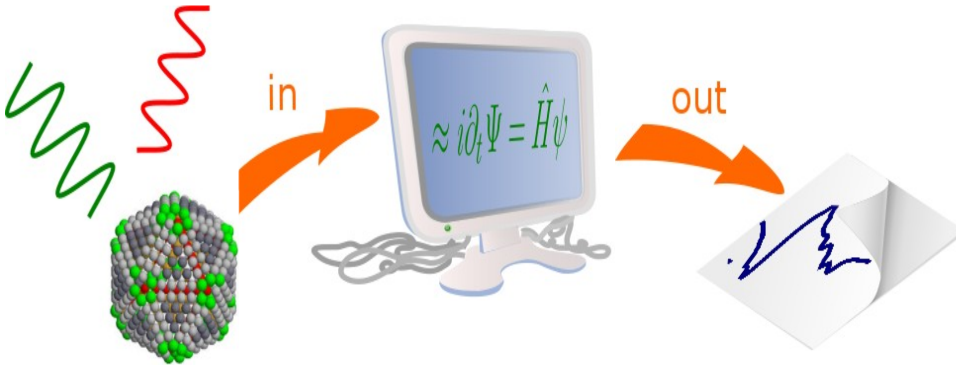


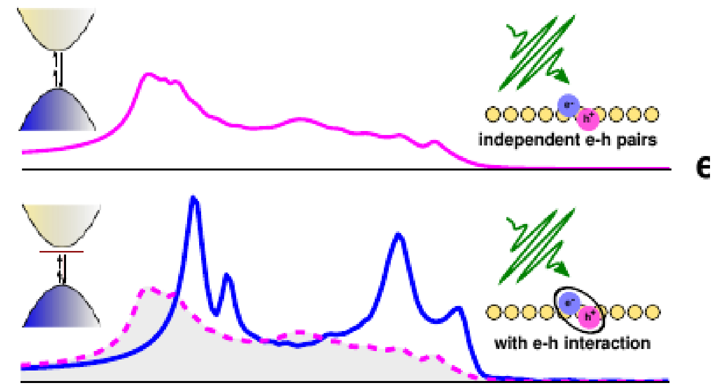


M. Grüning, **C. Attaccalite,** PRB-Rapid 88, 081102 (2014)

Non-linear spectroscopy

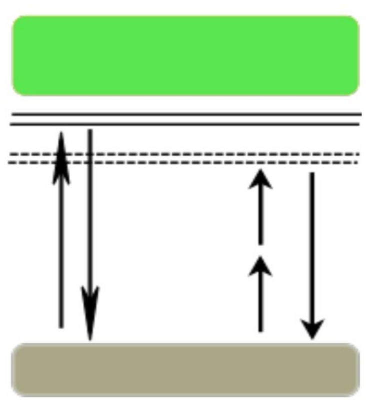
Second and third harmonic generation



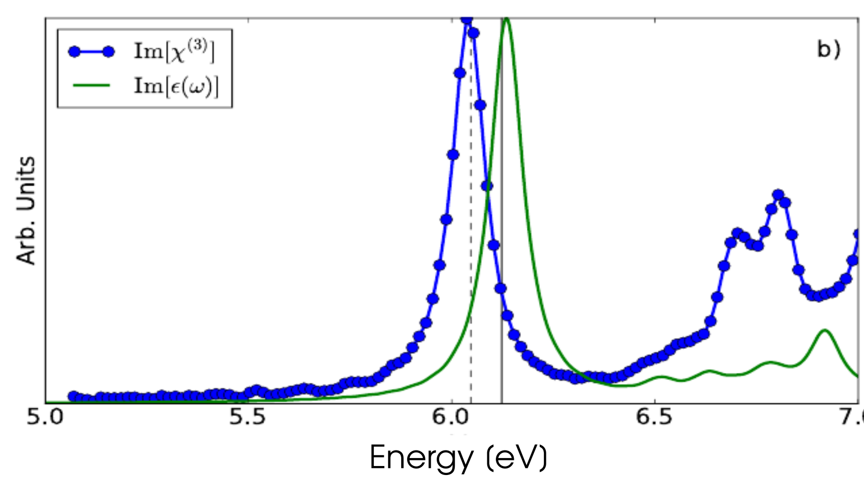


M. Grüning, **C. Attaccalite,** PRB-Rapid 88, 081102 (2014)

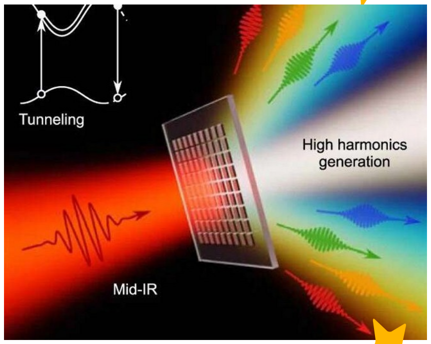
Two-photon absorption



Probing dark states

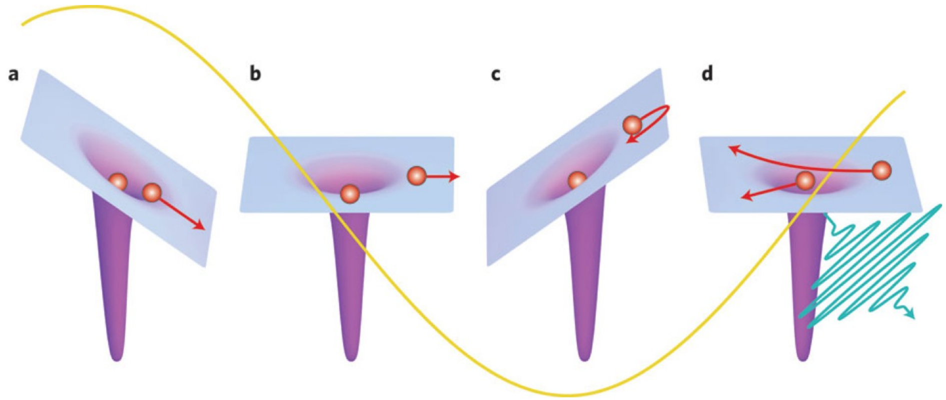


C. Attaccalite, M. Grüning, H Amara, S Latil, F Ducastelle, PRB 98 (16), 165126 (2018)



Design new optical high-harmonic generation devices

High-harmonic generation from gas to solids

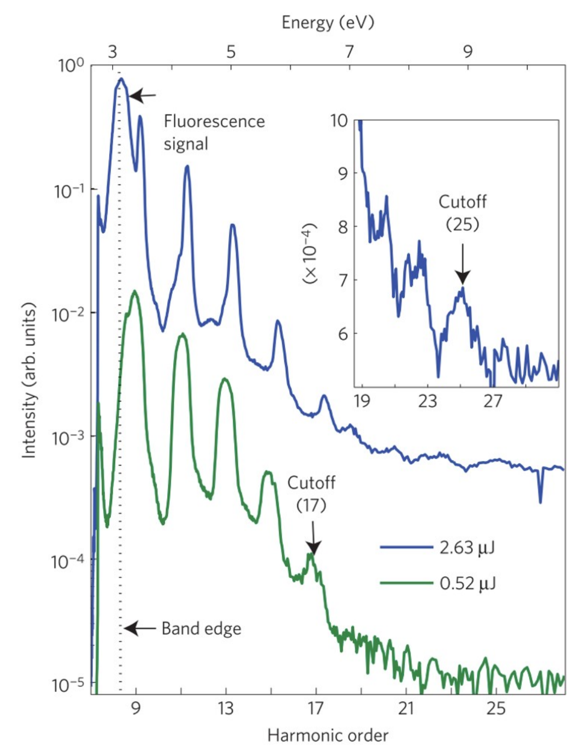


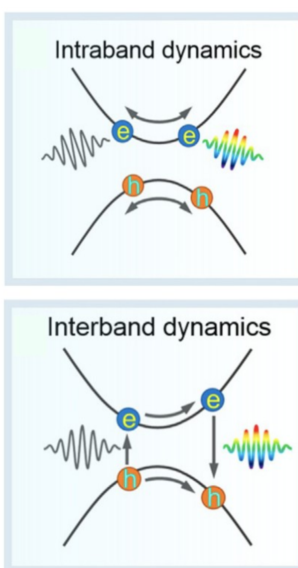
HHG in gases

Lewenstein PRA **49**, 2117 (1994)

HHG in solids

Nat Phys. **7**:138(2011)

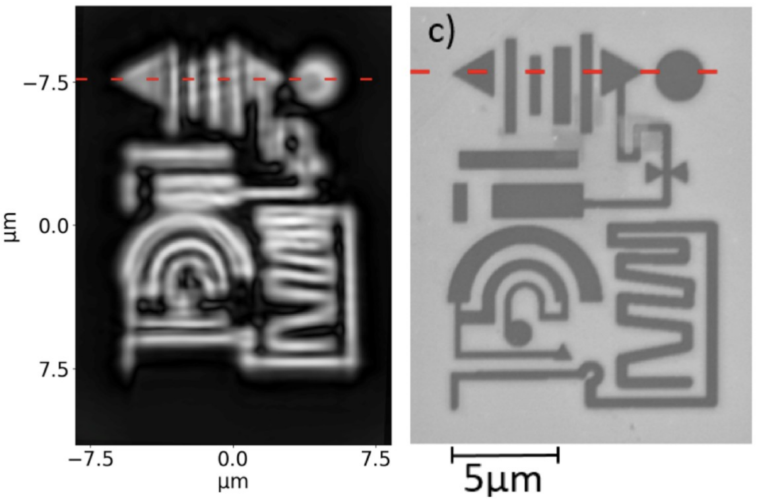




Why high-harmonic generation?

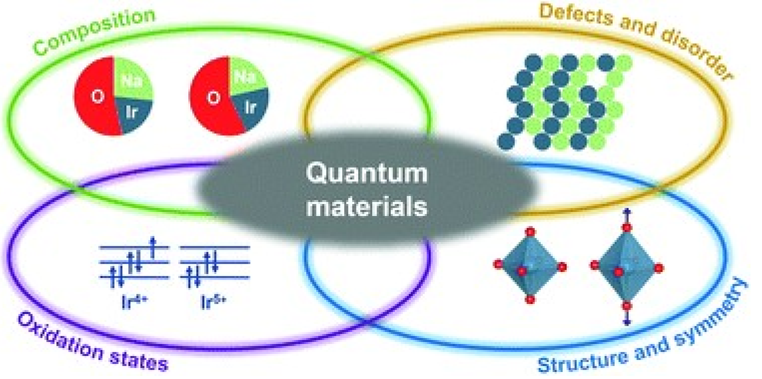
A Tool for materials' characterization:

tabletop lasers ranging from deep-UV to X-ray, high spatial resolution imaging , band structure reconstruction, time-resolved spectroscopy, time-resolved ARPES, phonon dynamics investigations

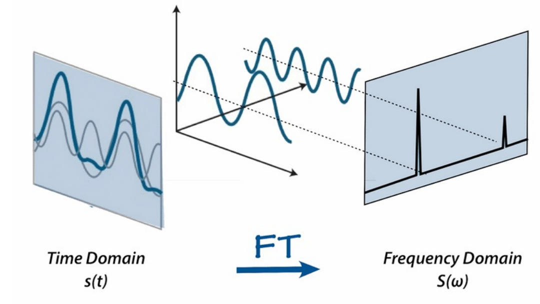


..and many open questions:

Excitons, correlation effects, topology
pump and probe, interfaces, tunability

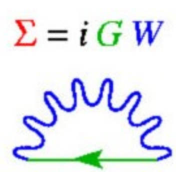


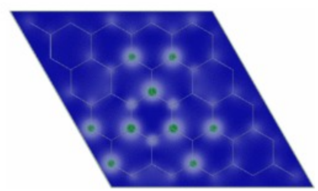
Real-time approach:

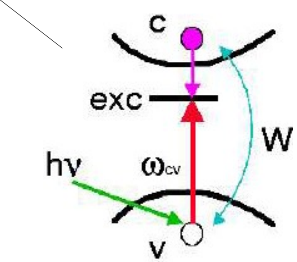


$$\left(\hat{H}^{\text{eff}}_{\mathbf{k}} - i\partial_t\right)|v_{\mathbf{k}n}\rangle = 0 \quad \longrightarrow \quad \mathrm{P} = \chi^{(1)}\mathcal{E} + \chi^{(2)}\mathcal{E}^2 + \chi^{(3)}\mathcal{E}^3 + \mathcal{O}(\mathcal{E}^4) \quad \xrightarrow{\mathscr{FT}} \quad \chi^{(2)}\ \chi^{(3)}$$

$$H^{eff} = h^0_k + \Delta h_k + V_H[\Delta\rho] + \Sigma_{sex}[\Delta\gamma]$$







- Berry-phase formulation for the PBCs
- Many-body effects can be included in an effective Hamiltonian
- Multiple lasers field can be simulated (pump and probe)

The Floquet formalism:

$$\left(\hat{H}^{\text{eff}}_{\mathbf{k}} - i\partial_t\right)|v_{\mathbf{k}n}\rangle = 0 \qquad |v_{\mathbf{k}n}\rangle = e^{-i\xi_{\mathbf{k}n}t} \sum_{\eta=-\infty}^{+\infty} e^{-i\eta\omega_0 t} \sum_i \widetilde{d}_{\mathbf{k}ni}(\eta)\,|\mu_{\mathbf{k}i}\rangle$$

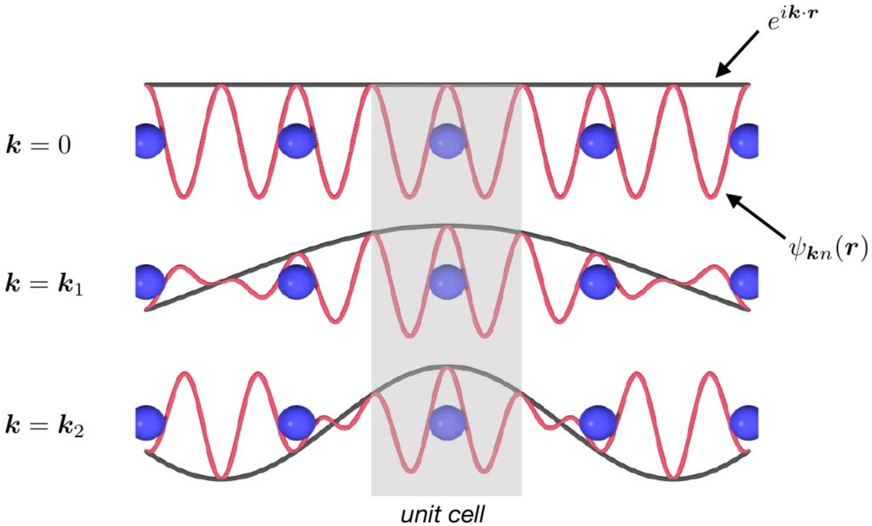
Time **independent** self-consistent eigen-problem

$$\sum_j^{+\infty} \sum_{\gamma=-\infty}^{+\infty} \Big[\underbrace{\left(E^{\text{IPA}}_{\mathbf{k}j} - \gamma\omega_0\right)\delta_{i,j}\delta_{\eta,\gamma}}_{\text{Diagonal}} + W_{\mathbf{k}ij}(\eta,\gamma)\Big]\,\widetilde{d}_{\mathbf{k}nj}(\gamma) = \xi_{\mathbf{k}n}\,\widetilde{d}_{\mathbf{k}ni}(\eta)$$

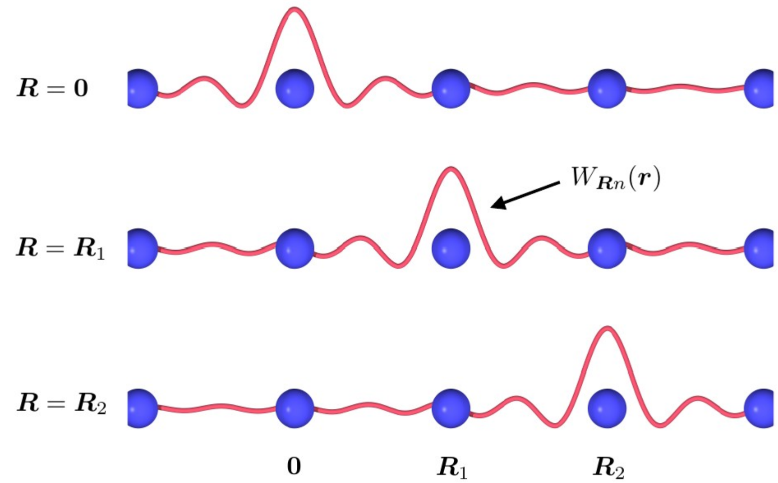
- Berry-phase formulation for the PBCs
- Many-body effects can be included in an effective Hamiltonian
- Lanzos-based solution of the eigenproblem
- Results analysis is much simpler

From ab-initio to models and beyond

Bloch functions



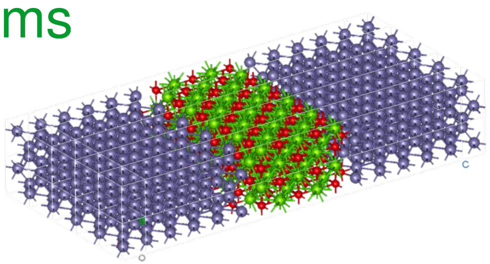
Wannier orbitals



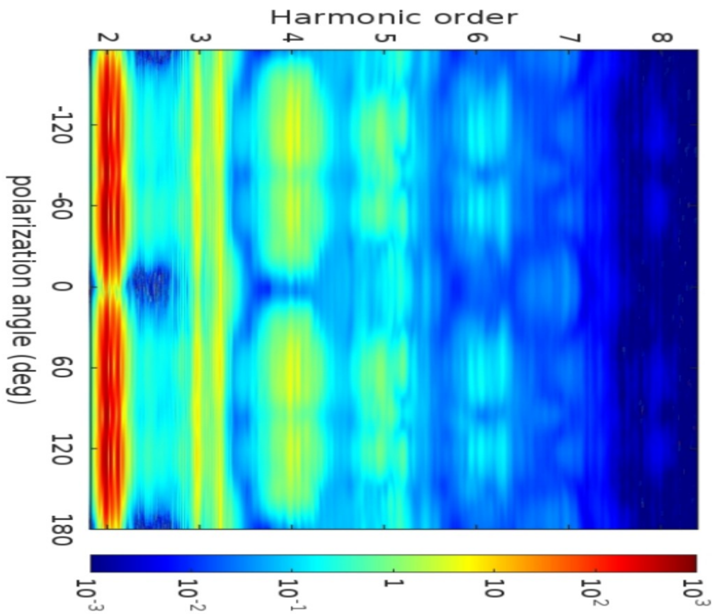
- Reformulate Floquet theory in Wannier basis
- We can start from simple models or build them using Wannier functions

$$H = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{ij} t_{ij} c_i^\dagger c_j + \dots$$

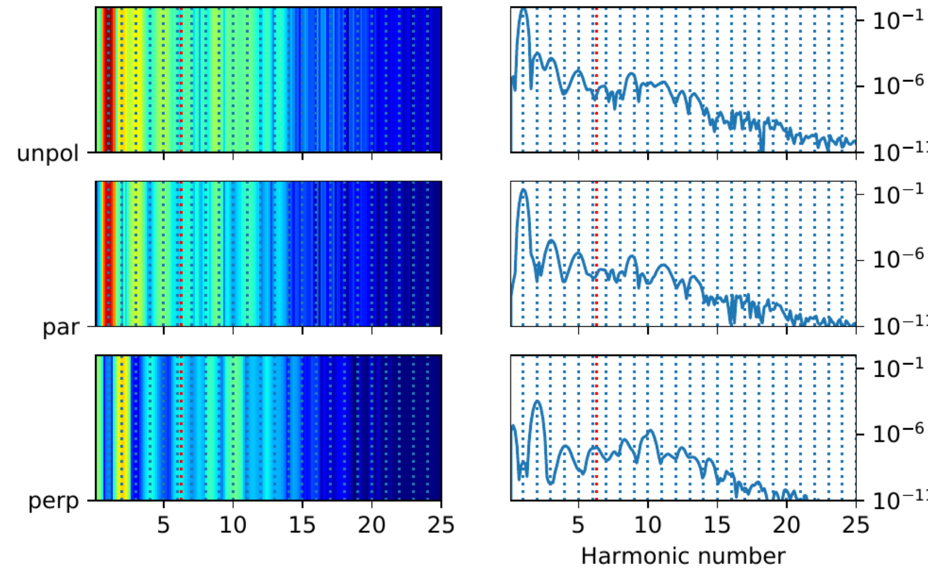
- Possibility to study non-periodic or complex systems (interfaces, surfaces)



Preliminary results

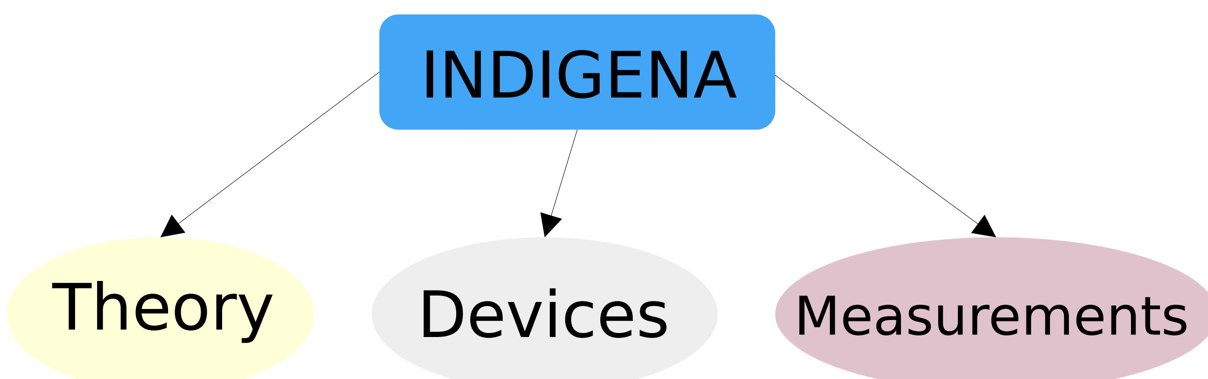


Validation in collaboration with
Caterina Vozzi in Milan(Italy)



HHG in ZnTe as a function
of polarization direction

Fundings



A*Midex
Initiative d'excellence Aix-Marseille

Scientific implication

Scientific Production ➡ **64** papers (6 PRL, 1 NanoLetter), **1** patent, more than **5000** citations, h-index **32**
19 invited talks

Supervision ➡ **4** PhD, **2** postdocs, **3** master, **2** internship

Teaching ➡ Statistical Mechanics (18/19),
Density Functional Theory(17/22/23)
9 International Schools(2008-)

Scientific research projects:

AGENCE NATIONALE DE LA RECHERCHE ANR

La Région Auvergne-Rhône-Alpes

HPC Europa

Aix*Marseille université Initiative d'excellence

GRAPHENE FLAGSHIP

cost European Cooperation in Science and Technology

Other projects:
Emergence CNRS
ETSF interships
PRACE

Service to the community

Editor fellow of SciPost

Membre du bureau du GDR REST

Membre du bureau du COST ACTION TUMIEE

Membre du Comité scientifique du GDR HOWDI et GDR-IRN HOWDI

Membre du bureau de la Division Matière Condensée de la SFP

Correspondant science ouverte du CINaM

Société Française de Physique

Conference Organization:

General meeting GDR-HOWDI and GDR-REST

4 Symposia/mini-colloque (PSI-k, SFP, etc...)

8 Conferences/Workshop (ETSF, Gutwiller, ….)

2 Schools

2 Year Weekly seminars at CINaM and ETSF online seminars

CV

Non-linear-optics
Electron-phonon
Code developement

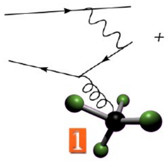
Project

High-harmonic
generation
first principles calculations
and modelling

Thanks!

Any questions?

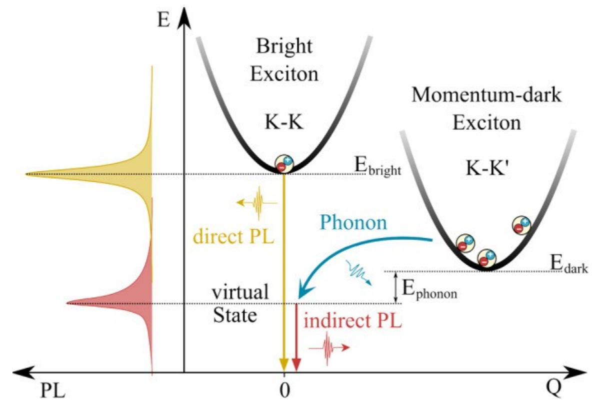
Expected results



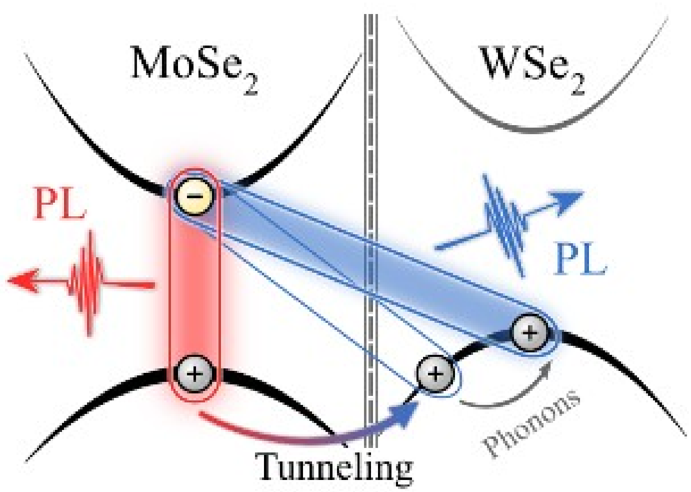
Exciton-phonon Hamiltonian

$$\mathcal{H}_{\mathrm{el-ph}} = \sum_{kq\mu} \mathrm{M}^{\mu}_{kq} (v^{\dagger}_{k+q} v_k - u^{\dagger}_{k+q} u_k)(a_{q\mu} + a^{\dagger}_{-q\mu})$$

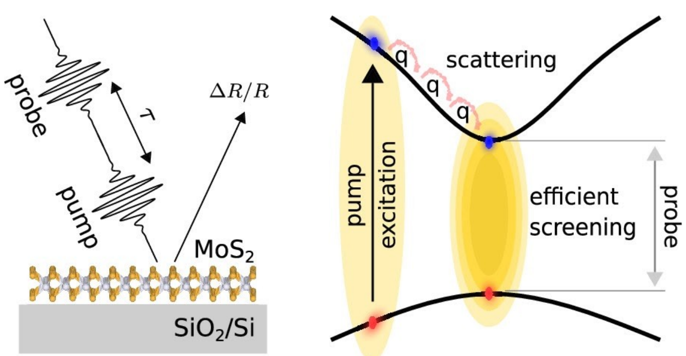
Phonon-assisted luminescence



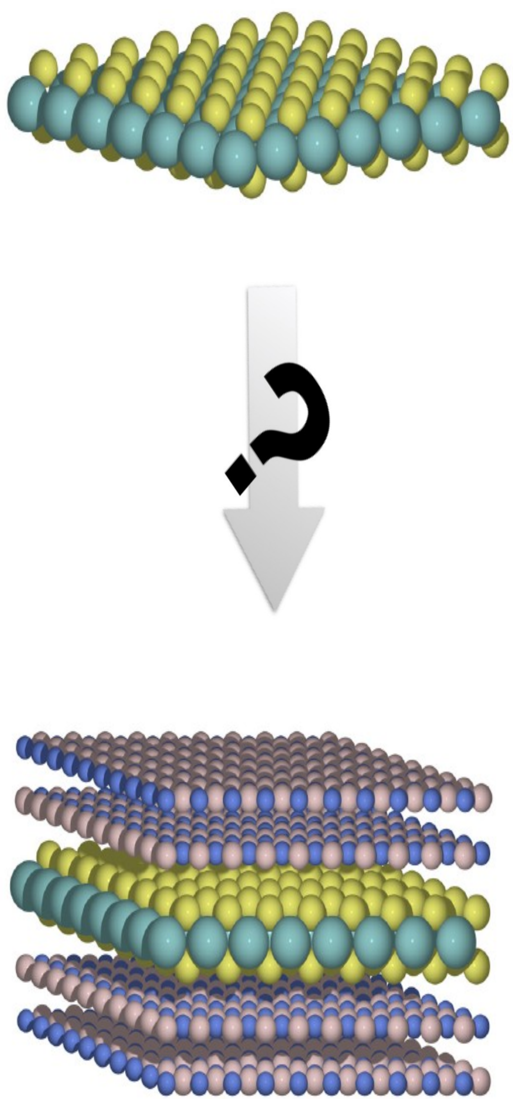
Exciton dynamics

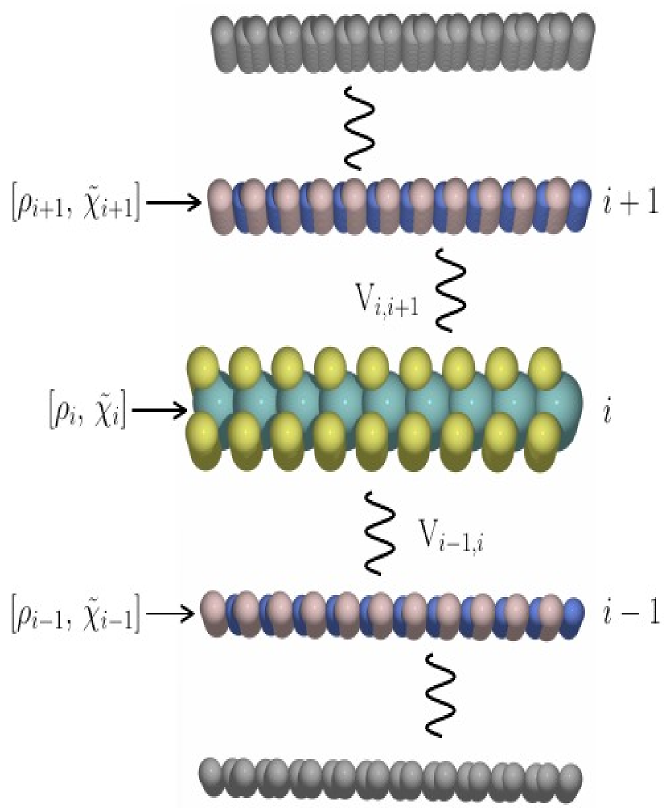


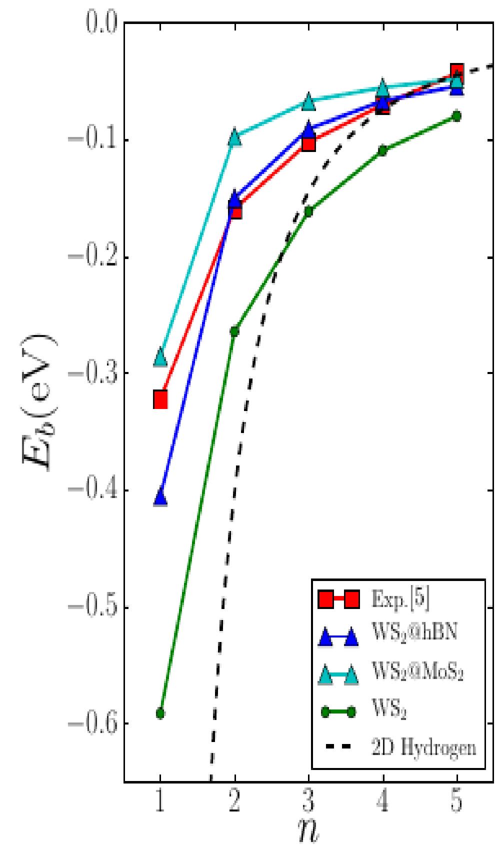
Pump-probe



Quantum Electrostatic Heterostructure model and its relatives

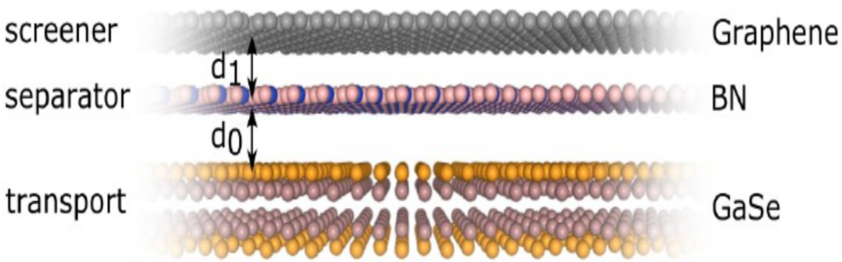


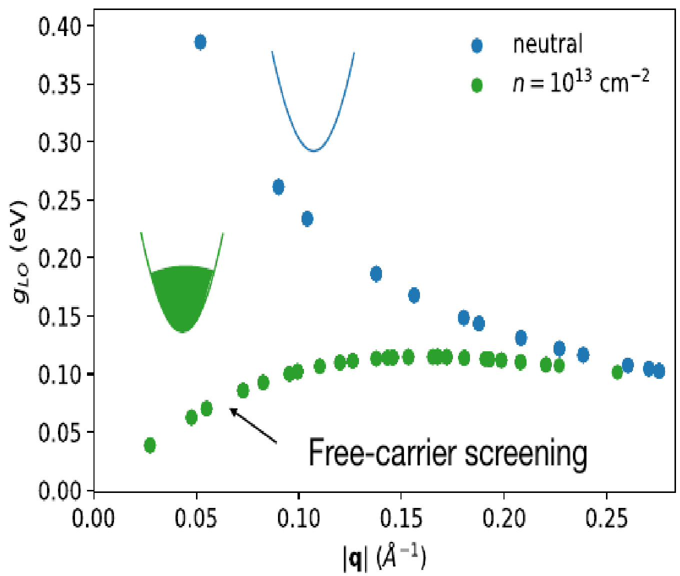


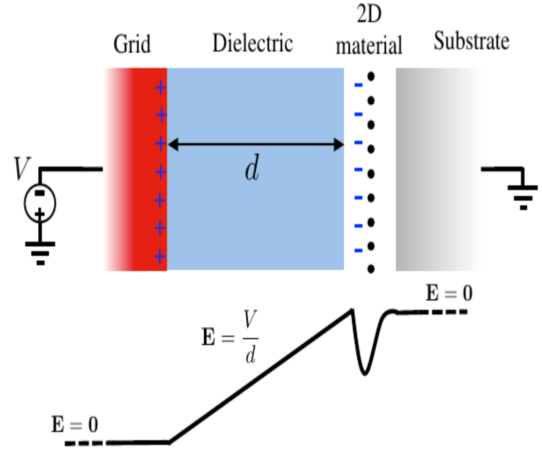


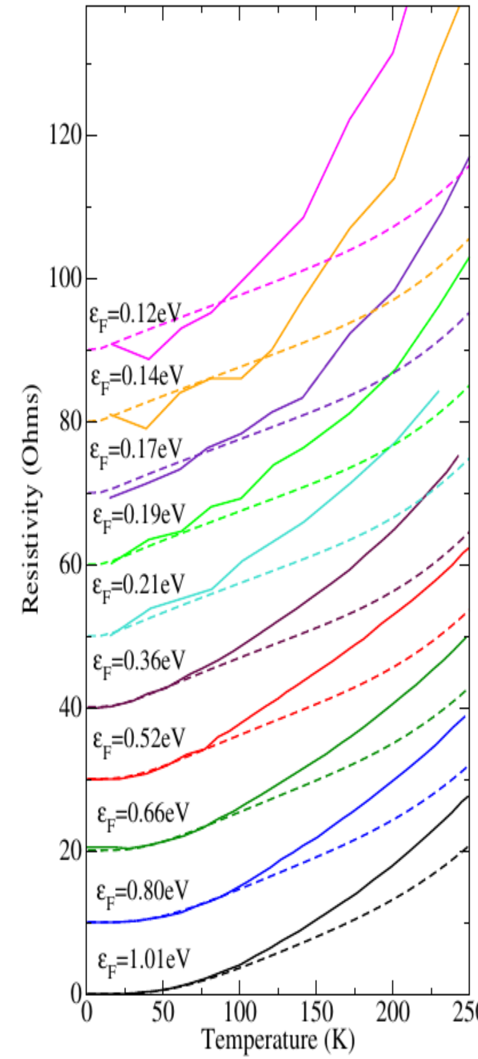
K. Andersen, S. Latini and K.S. Thygesen, Nanoletter, **15**, 4616 (2015)
L. Sponza, F. Ducastelle, https://arxiv.org/abs/2011.07811

Environment: phonons



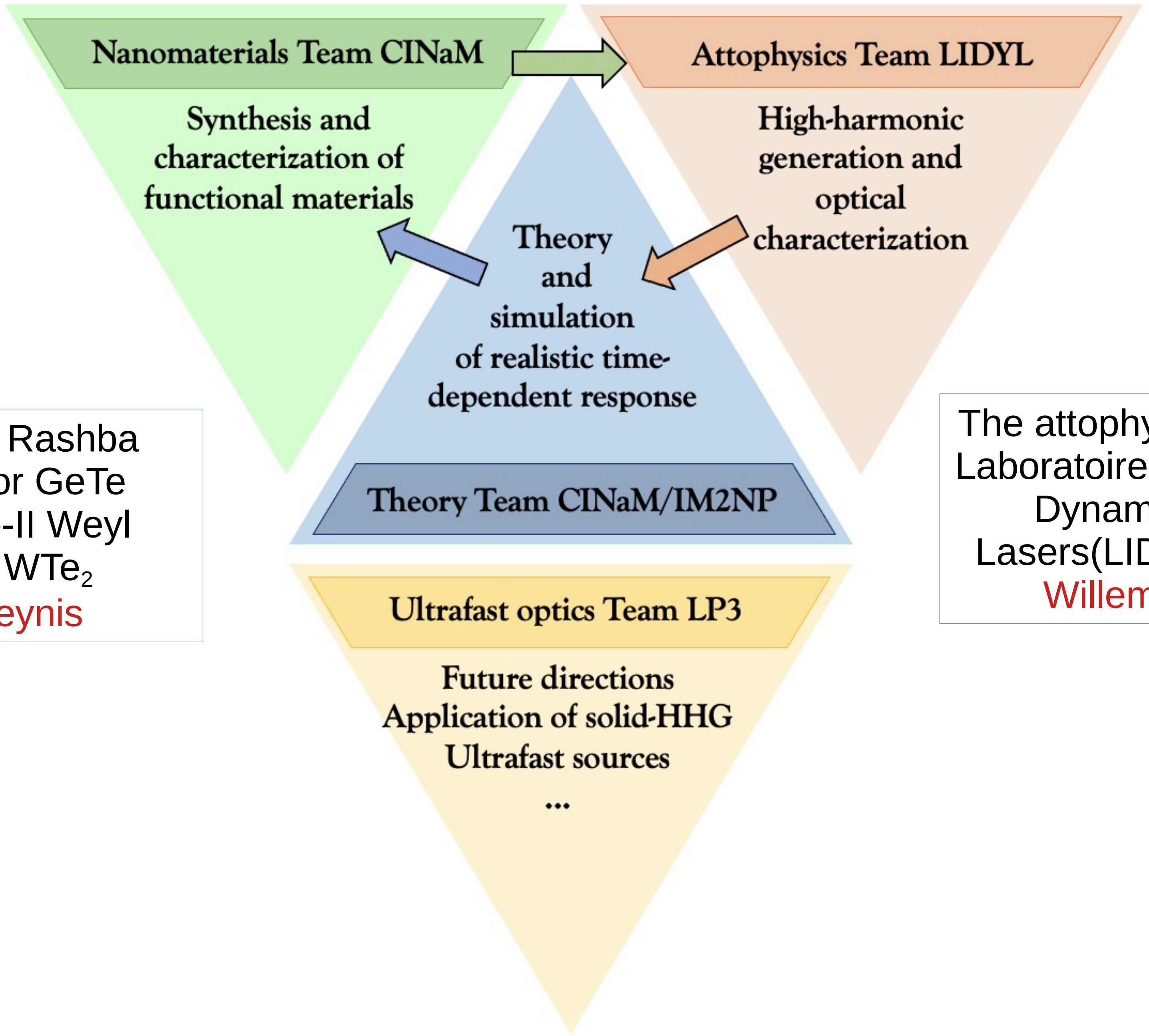






T. Sohier, et al. Phys. Rev. Mat. **5**, 024004 (2021)

Indigena



Ferroelectric Rashba semiconductor GeTe and the type-II Weyl semimetal WTe_2

Fabien Cheynis

The attophysics team at Laboratoire Interactions, Dynamiques et Lasers(LIDL) (Saclay)

Willem Boutu