Scientific report on the *20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods*

University of the Basque Country, San Sebastián, Spain
8th-10th January 2020

Organizers: Ion Errea (University of the Basque Country), Aran Garcia-Lekue (Donostia International Physics Centre), and Ivo Souza (University of the Basque Country).

Funding: Psi-k, Donostia International Physics Centre, Simune Atomistics, Basque Government. Logistical support was provided by the University of the Basque Country.

Workshop website: http://totalenergy2020.dipc.org/

Introduction

This event was the latest in the “mini” series associated with the “Total Energy and Force Methods” workshops, held at ICTP in Trieste every two years. Since 1987 the Trieste workshops have taken place in odd-numbered years, alternating with the mini workshops, held each even-numbered year in a different location. The most recent workshops of the mini series took place in Madrid (2000), Tenerife (2002), Paris (2004), Cambridge (2006), Bonn (2008), Shanghai (2010), Barcelona (2012), Lausanne (2014), Luxembourg (2016), and Cambridge (2018).

The workshop focused on the most recent developments in the field of electronic structure methods from the first-principles perspective, their diverse applications and mathematical foundations. The numerous approaches that are developed and used in the electronic-structure community provide the foundation for computing many physical and chemical properties of solids, liquids, and low-dimensional systems. However, there are numerous challenging applications for which the level of approximation is insufficient or where computational costs are prohibitive for accurate quantitative prediction of material properties. Therefore, continued efforts are devoted to the improvement of existing methods, and the development of new methods.

Description

The participants arrived at the auditorium of the Carlos Santamaría Centre (the university's Main Library), on Wednesday 8th January at 8:15 for registration. At 8:45, Prof. Ion Errea welcomed the participants and introduced the workshop format: nine sessions consisting of two or three 30-minute talks, each followed by 10 minutes of Q&As. In total, there were 23 invited talks spread over 2.5 days. The talks were streamed live on the Internet, as announced on the Psi-k mailing list on January 7th 2020. Most of the lectures recorded are available online at http://dipc.tv/kategoria.php?lang=en&idkategoria=0&ordenatua=&bilaketa_testua=Mini%202020&hurrengoa=0 .

In the evening of the first day, a Poster Session was held in the Engineering School, where 63 posters were presented. A poster prize, sponsored by **Simune Atomistics** (a startup located in San Sebastián), was awarded to two poster presenters, Sofia Sanz and

Ke Liao, during the conference dinner at the end of the second day, which was held at the Ni Neu restaurant.

The abstracts of the talks and posters, as well as the list of participants, can be found in the workshop's Book of Abstracts (also attached to this report). In total, there were 122 registered participants from all over the world, supplemented by numerous local participants.

Scientific topics covered:

- Electron-phonon coupling
- Nonlinear elastic and optical responses of dielectrics
- 2D materials
- Correlation effects
- Superconductivity
- Topological materials
- Transport properties
- Excitations
- DFT for cavity QED
- Biophysics

List of invited speakers

Here is the final list of invited speakers:

Antia Botana,Arizona State University (USA)
Matthew Foulkes, Imperial College London (UK)
Xavier Gonze, Université Catholique de Louvain (Belgium)
Myrta Grüning, Queen's University Belfast (UK)
Efthimios Kaxiras, Harvard University (USA)
Eduard Matito, Donostia International Physics Center (Spain)
Miguel Marques, Martin-Luther-University Halle-Wittemberg (Germany)
Lorenzo Monacelli, Sapienza University of Rome (Italy)
Titus Neupert, University of Zurich (Switzerland)
Thomas Olsen, Technical University of Denmark (Denmark)
Nick Papior, Technical University of Denmark (Denmark)
Silvia Picozzi, Università degli Studi di Chieti (Italy)

Cheol-Hwan Park, Seoul National University (South Korea)
Andrew M. Rappe, University of Pennsylvania (United States)
Alexandre R. Rocha, State University of São Paulo (Brazil)
Ivana Savic, Tyndall National Institute (Ireland)
Thibault Sohier, Ecole Polytechnique Fédérale de Lausanne (Switzerland)
Massimiliano Stengel, Institut de Ciència de Materials de Barcelona (Spain)
Ilya Tokatly, University of the Basque Country (Spain)
Roser Valentí, Goethe University Frankfurt (Germany)
Xiangang Wan, Nanjing University (China)
Binghai Yan, Weizzmann Institute of Science (Israel)
Jakub Zelezny, Czech Academy of Sciences (Czech Republic)

Program

The full program of the workshop was the following.

Wednesday 8		
8:15-8:45	Registration	
8:45-9:00	Opening remarks	
Session 1, Chair Ion Errea		
9:00-9:40	Gonze	Predominance of non-adiabatic effects in zero- point renormalization of electronic energies
9:40-10:20	Savic	Electron-phonon coupling and thermoelectric transport in PbTe from first principles
10:20-11:00	Monacelli	Dynamical propagation of quantum nuclei in solids: from arharmonic Raman&IR to out of equilibrium phenomena. Applications to high- pressure hydrogen
11:00-11:30	Coffee-break	
Session 2, Chair Erik Koch		
11:30-12:10	Stengel	First-principles theory of flexoelectricity and related materials properties
12:10-12:50	Grüning	Nonlinear optics from first-principles real-time approaches
13:00-15:00	Lunch	
Session 3, Chair Nicola Marzari		
15:00-15:45	Olsen	The computational 2D materials database: high throughput screening for topological and ferromagnetic 2D materials
15:40-16:20	Park	Electronic structure of two-dimensional antiferromagnetic transition-mtal phosphorus trisulfides
16:20-17:00	Sohier	Phonon-limited transport in 2D materials
17:30-19:30	**Poster Session**	

Thursday 9		
Session 4, Chair Emilio Artacho		
9:00-9:40	Rappe	TBA
9:40-10:20	Foulkes	Ab-initio solutions of the many-electron Schrödinger equation with deep neural networks
10:20-11:00	Matito	Singling out dynamic and nondynamic correlation
11:00-11:30	Coffee-break	
Session 5, Chair Ilya Tokatly		
11:30-12:10	Valentí	Strain effects in Fe-based superconductors: nematicity, exotic magnetism and superelasticity
12:10-12:50	Botana	Low-valence layered nickelates: a cuprate analog for high-temperature superconductivity?
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15:00-15:45	Neupert	A topological tour through momentum space in memory of Alexey Soluyanov
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Session 7, Chair Pablo Ordejón		
17:30-18:10	Kaxiras	Twistronics: electron localization in stacked layers of 2D materials
18:10-18:50	Picozzi	Towards ferroics in 2-dimensions
20:30	**Conference Dinner**	

Friday 10		
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12:50-13:00	Closing Remarks	

Workshop on Computational Physics and Materials Science:

Total Energy and Force Methods 2020

Donostia-San Sebastián, Spain

January 8-10, 2020

Institutional support and funding

DIPC
Donostia International Physics Center

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Universidad del País Vasco
Euskal Herriko Unibertsitatea

cecam
Centre Européen de Calcul Atomique et Moléculaire

ZCAM
Zaragoza Scientific Center for Advanced Modeling

Universidad Zaragoza
1542

SIMUNE
ATOMISTIC SIMULATIONS

Preface

This workshop is organized within the well-established “Total Energy and Force” conference series, which is held at ICTP in Trieste every odd year, and at a different place in the world every even year. The previous most recent workshops of this series outside Trieste took place in Barcelona (2012), Lausanne (2014), Luxembourg (2016) and Cambridge (2018).

The main objective of this event is to identify new developments and topics in the field of electronic-structure methods from the first-principles perspective, their diverse applications, and its mathematical foundations. As such, it provides a great opportunity to assemble a wide range of leading scientists working on different aspects of computational material science.

The workshop aims to cover the following topics:

- Electron-phonon
- Dielectrics
- 2D materials
- Correlation effects
- Superconductivity
- Topological materials
- Transport properties
- Excitations

Organizing committee

- **Aran Garcia-Lekue**, Donostia International Physics Center
- **Ivo Souza**, University of the Basque Country
- **Ion Errea**, University of the Basque Country

Scientific advisory board

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- **W. Andreoni**, Ecole Polytechnique Fédérale de Lausanne
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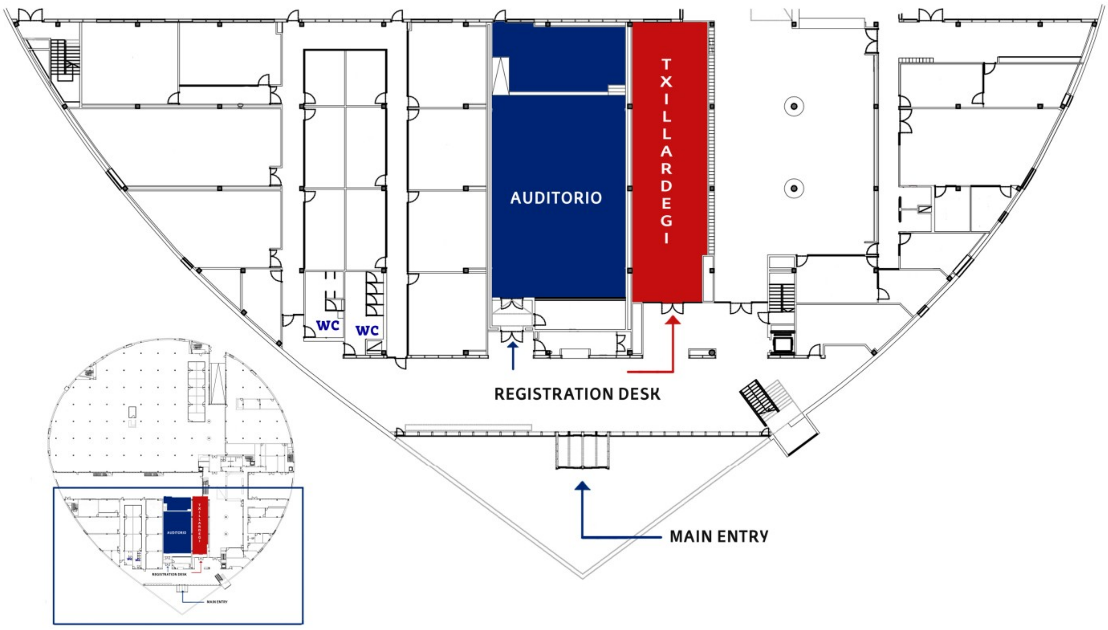
- **M. Finnis**, Imperial College
- **R. Gebauer**, International Centre for Theoretical Physics
- **X.-G. Gong**, Fudan University
- **J. Ihm**, Seoul National University
- **E. Koch**, Forschungszentrum Jülich
- **G. Kresse**, University of Vienna
- **R. M. Martin**, Stanford University
- **F. Mauri**, University "La Sapienza"
- **A. Mostofi**, Imperial College London
- **S. Narasimhan**, JNCASR Bangalore
- **J. B. Neaton**, Lawrence Berkeley National Labs
- **W. Pickett**, University of California, Davis
- **A. Rappe**, University of Pennsylvania
- **L. Reining**, Ecole Polytechnique Palaiseau
- **G.-M. Rignanes**e, Université Catholique de Louvain

Conference locations

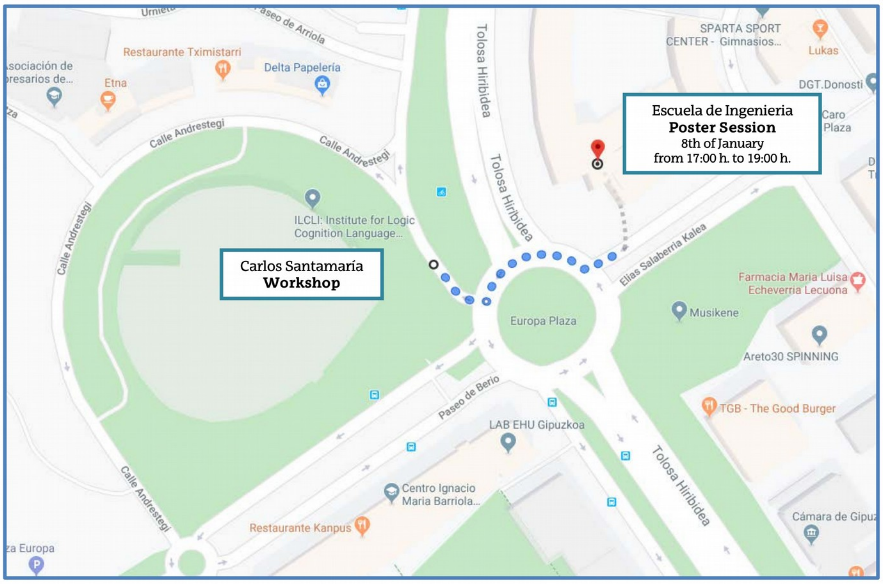
Conference venue: Carlos Santamaría Centre

Elhuyar Plaza 2, Donostia/San Sebastián



Poster session: Escuela de Ingeniería de Gipuzkoa

Europa Plaza 1, Donostia/San Sebastián


Escuela de Ingenieria
Poster Session
8th of January
from 17:00 h. to 19:00 h.

Carlos Santamaría
Workshop

Conference dinner: “Ni Neu” Restaurant

Zurriola Hiribidea 1, Donostia/San Sebastián

Dinner:
Ni Neu restaurant,
Zurriola Hiribidea 1

Workshop venue:
Carlos Santamaría UPV/EHU
library

Wifi information

Network: EHU-wGuest

Login: energy20

Password: energy20

Scientific programme

Invited talks: 30 min. talk + 10 min. discussion

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Poster session

P1	Aguado	GW study of pressure-induced topological insulator transition in group IV-tellurides
P2	Artyukhin	Towards phase diagrams of $IrTe_2$ from first principles
P3	Aschauer	Self-consistent site-dependent DFT+U(+V) for defects
P4	Aseginolaza	Anharmonic renormalization of flexural acoustic modes in graphene
P5	Baumeister	Towards a faster and simpler PAW method
P6	Belli	Quantum anharmonic effects on the superconducting LaH_{10}
P7	Belviso	Electrical tuning of vibrational modes in transition metal dichalcogenides
P8	Bennet	Competition between structural and electronic phase transitions in perovskite thin films
P9	Bianco	Quantum enhancement of charge density wave in NbS_2 in the 2D limit
P10	Bolen	Electronic transport in $Mo_2ScC_2O_2$ MXene
P11	Bouchakri	Theoretical study in DFT of bi- metallic compounds of transition metals with cyclic ligand
P12	Brandimarte	Deciphering the electronic structure of 5-armchair graphene nanoribbons and its topological end-states
P13	Corona-Garcia	Structural and electronic properties of puckered-buckled arsenene lateral heterostructures
P14	Da Pieve	Multiscale modeling of radiation effects on biological matter and functional materials for missions to Mars
P15	Das B.K.	Band gap modulation of dynamically stable bilayer and trilayer WS_2 configurations under external field
P16	Das T.	Band gap of 3D metal oxides and quasi-2D materials from hybrid density functional theory
P17	D. de Cerio	Electronic structure optimization of nanoporous graphene
P18	Durgun	Characterization and stability of Janus TiXY (X/Y=S, Se and Te) monolayers
P19	Eleno	Controlling type-II Dirac semimetal $NiTe_2$ electronic and elastic properties via strain and alkaline-element intercalation
P20	Forcellini	Electronic stopping power using Floquet theory: examples and applications
P21	Garai-Marin	Ab-initio study of the electron- phonon interaction of a single Fe adatom on the MgO/Ag(100) surface
P22	G. de Gurtubay	Magnetic oscillations induced by phonons in non-magnetic materials
P23	Gavin	Simulation protocols for paramagnetic transition-metal oxides
P24	Goikoetxea	3d transition metal oxide chains: spin-phases, magnetic exchange coupling and anisotropy
P25	Gu	Electronic stopping power for protons in liquid water from TDDFT simulations with geometry pre-sampling

P26	Guerra	Ab-initio modeling of materials properties: an application to thermoelectric magnesium silicide alloys
P27	Gutierrez Amigo	Phonon topology on the buckled honeycomb lattice
P28	Heid	Density functional perturbation theory with DFT+U in the mixed-basis framework
P29	Hutcheon	Exchange-diffusion Monte Carlo
P30	Ibañez-Azpiroz	Directional shift current and dipole selection rules in mirror-symmetric BC_2N
P31	Iraola	Topological semimetals with butterfly-like four-point intersecting ellipses
P32	Khanh	Accurate methods for the description of binding energies of molecular solids
P33	Kim	TBFIT: an open-source software package for Slater-Koster tight- binding parameter fitting
P34	Koval	Electronic stopping power for protons in solar-cell materials from first-principles calculations
P35	Kretz	Assessment of optimally-tuned range-separated hybrid functionals for the calculation of excited state properties in organic dyes
P36	Kuklin	Proximity and defect induced band gap renormalization in 2D $PdSe_2$
P37	Lei	Computational attempts to approach magnetism in metal-organic frameworks (MOFs)
P38	Li	Control of spintronic properties of bimetallic MXenes via surface functionalization
P39	Liao	A comparative study using state-of-the-art electronic structure theories on solid hydrogen phases under high pressures
P40	Majumdar	Strong multi-layer dependency of exothermic dissocation in polymeric nitrogene: Towards high energy density inorganic materials
P41	Menchón	DFT exploration of magnetic properties in substitutionally doped graphene nanoribbons
P42	Meninno	Ab initio study of possible metastable occupation of tetrahedral sites in Palladium Hydride compounds
P43	Missaoui	Molecule contamination effects on nanofriction in layered materials: an ab initio study
P44	Mitxelena	A functional for strong correlation in 1D&2D
P45	Muñoz Saez	PyProcar: a python library for electronic structure pre/post-processing
P46	Muñoz-Santiburcio	Excitation dynamics in proton- irradiated ice
P47	Nakhaee	Tight-binding studio: a technical software application to find the parameters of tight-binding Hamiltonian
P48	Necio	An ab-initio investigation of a 2D magnet in the presence of graphene
P49	Plekhanov	Controlling the properties of the correlated materials
P50	Ponce	Predictive calculations of phonon-limited carrier mobilities in semiconductors
P51	Rappe	A general approach towards continuous translational symmetry in finite difference real-space calculations

P52	Rauch	Local mixing in modified Becke-Johnson potential for low-dimensional systems
P53	Robredo	Straining the 3fold: hall viscosity of a new Fermion
P54	Rybkin	Density functional embedding theory in gaussian and plane waves formalism
P55	Sanz	N-terminal graphene-based nanostructures for electron quantum optical setups
P56	Song	Lattice dynamics of Cubic $SrTiO_3$: a simple way of temperature-dependent phonon calculations
P57	Sotoudeh	Theoretical study of multivalent ionic transport in spinel host materials
P58	Tsirkin	Wannier19: an advanced tool for interpolation of Berry curvature and related quantities
P59	Tsumuraya	Stability of π-electron-deuterium coupled ordering in hydrogen-bonded molecular conductors κ-D_3 (Cat-EDFT-TTF/ST)$_2$
P60	Vanzan	Computational insight on the energy transfer properties of small noble metal nanoclusters
P61	Woods	Computing the self-consistent field in Kohn-Sham density functional theory
P62	Yazyev	Understanding atomic and electronic structure across the family of 2D transition metal dichalcogenides
P63	Zubeltzu	Theoretical approach to II-VI nanoclusters in ionic liquids

Wednesday January 8

Predominance of non-adiabatic effects in zero-point renormalization of electronic energies

X. Gonze[1,2], A. Miglio[1], V. Brousseau-Couture[1,3], G. Antonius[4,5], Y.-H. Chan[4], S.G. Louie[4], M. Giantomassi[1] and M. Côté[3]

[1]Institute of Condensed Matter & Nanosciences, UCLouvain, Belgium.
[2]Skolkovo Institute of Science and Technology, Moscow, Russia.
[3]Dept. de Physique, U. de Montréal, Montréal, Canada.
[4]Dept. of Physics, U. California at Berkeley, CA, USA and Materials Sciences Div., NBNL, Berkeley, CA, USA.
[5]Dept. de Chimie, Biophysique et Physique, U. Québec à Trois-Rivières, Trois-Rivières, Canada.

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Electronic and optical properties of materials are affected by atomic motion through electron-phonon interaction. This interaction had two noticeable effects on the electronic structure: variation of band gaps with temperature, but also band-gap renormalization even at zero temperature, due to zero-point motion. Ignored in most calculations of the electronic structure, zero-point effects have been evaluated recently from first principles for several materials. Many of these calculations relied on the adiabatic approximation, reasonably valid for materials without infrared activity, but eagerly applied to other materials.
We present the first large-scale (29 materials) first-principles evaluation of band edge zero-point renormalization (ZPR) beyond the adiabatic approximation [1]. For materials with light elements, the band gap renormalization is often larger than 0.3 eV and up to 1.1 eV. This effect cannot be ignored if accurate band gaps are sought. In particular, we show that it is useless to go beyond G0W0 without including ZPR effects in such materials. For infrared-active materials, global agreement with available experimental data is obtained only when nonadiabatic effects are taken into account. They even dominate zero-point renormalization for many materials. We present a generalized Fröhlich model (multiphonon, anisotropic and degenerate electronic extrema) that represents accurately non-adiabatic effect, and assess its accuracy against first-principles results. This model describes the essential physics and accounts for more than half the total ZPR for a large set of materials, especially for valence band edges, despite its neglect of interband electronic transitions, Debye-Waller contributions and acoustic phonon contributions present in the full first-principles approach. By the same token, the domain of validity of hypotheses underlying the Fröhlich model, used for decades, is established.

[1] A. Miglio, V. Brousseau-Couture, G. Antonius, Y.-H. Chan, S.G. Louie, M. Giantomassi, M. Côté, and X. Gonze. Submitted for publication.

Electron-phonon coupling and thermoelectric transport in PbTe from first principles

I. Savic[1]

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I will describe our recent development of a first principles thermoelectric transport model based on the Boltzmann transport equation [1,2], which goes beyond the current state-of-the-art approaches [3] in certain aspects. Best performing thermoelectric materials like PbTe and Bi2Te3 typically have narrow band gaps, which are usually underestimated using the standard approximations for the exchange-correlation energy in density functional theory. This may lead to the inaccurate description of the curvatures of the conduction and valence bands near the band gap, as well as the inaccurate description of corresponding electron-phonon matrix elements. Furthermore, in narrow gap semiconductors, the conduction and valence bands near the gap can be strongly renormalized by temperature. Here I will show that our model can straightforwardly incorporate these effects using the example of PbTe[4,5].

Regarding the physical effects, I will show that soft transverse optical modes are the key to the high thermoelectric figure of merit of PbTe: they preserve its high electronic conductivity while suppressing the lattice thermal conductivity [1]. Our results also illustrate that the actual band gap values in PbTe are very close to the predicted optimum values in a broad range of temperatures, which also contributes to the large thermoelectric figure of merit [2].

[1] J. Cao, J. D. Querales-Flores, A. R. Murphy, S. Fahy, and I. Savic, Phys. Rev. B, 98, 205202 (2018)
[2] J. Cao, J. D. Querales-Flores, S. Fahy, and I. Savic, arXiv:1906.05322
[3] S. Ponce, E. R. Margine, C. Verdi, and F. Giustino, Comput. Phys. Commun. 209, 116 (2016)
[4] A. R. Murphy, F. Murphy-Armando, S. Fahy, and I. Savic, Phys. Rev. B 98, 085201 (2018)
[5] J. D. Querales-Flores, J. Cao, S. Fahy, and I. Savic, Phys. Rev. Materials 3, 055405 (2019)

Dynamical propagation of quantum nuclei in solids: from anharmonic Raman&IR to out of equilibrium phenomena. Applications to high-pressure hydrogen.

L. Monacelli[1,2], I. Errea[3,4,5], M. Calandra and F. Mauri[1,2]

[1]University of Rome "Sapienza", Physics departement
[2]Italian Institute of Technology, Graphene Flagship
[3]Fisika Aplikatua 1 saila, Gipuzkoako Ingeniaritza Eskola
[4]Centro de Física de Materiales (CSIC-UPV/EHU)
[5]University of the Basque Country (UPV/EHU)

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Vibrational spectroscopy is one of the main experimental tools to explore condensed matter theory. It is relatively easy to use and the experimental apparatus required is commonly available in modern laboratories. However, the interpretation of the results relies mostly on the harmonic approximation. This hypothesis breaks down in materials close to structural instabilities, as ferroelectrics[1] or transition metals dycalcogeneids[2]. Moreover, systems with light atoms experience strong fluctuations induced by quantum zero-point motion, which must be treated anharmonically to get quantitative predictive results. It is the case of high-pressure hydrogen and hydrates[3- 5].

In this talk, I will introduce a new theoretical framework to deal with nuclear motion with quantum fluctuations and anharmonicities. This theory is time-dependent: it allows simulating dynamical properties as full anharmonic IR and Raman spectra and out-of-equilibrium processes. It maintains the computational cost of a standard molecular dynamics simulation.

I apply this new theory to predict the Raman and IR spectrum of high-pressure phase III of hydrogen, comparing to the experimental data. The results obtained unveil an unprecedented accuracy in this system. They enable ab-initio simulations to be predictive with a relatively small computational effort, opening the way to solve the long-standing experimental debates on high-pressure hydrogen phase-diagram.

[1] Aseginolaza, Unai, et al. "Phonon collapse and second-order phase transition in thermoelectric SnSe." Physical review letters 122.7 (2019)

[2] Bianco, Rafaello, et al. "Quantum Enhancement of Charge Density Wave in NbS2 in the Two-Dimensional Limit." Nano letters 19.5 (2019): 3098-3103

[3] Errea, Ion, et al. "High-pressure hydrogen sulfide from first principles: A strongly anharmonic phonon-mediated superconductor." Physical review letters 114.15 (2015)

[4] Borinaga, Miguel, et al. "Anharmonic enhancement of superconductivity in metallic molecular Cmca−4 hydrogen at high pressure: a first-principles study." Journal of Physics: Condensed Matter 28.49 (2016)

[5] Errea, Ion, et al. "Quantum Crystal Structure in the 250 K Superconducting Lanthanum Hydride." arXiv preprint arXiv:1907.11916 (2019).

First-principles theory of flexoelectricity and related materials properties

Massimiliano Stengel[1,2]

[1]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), 08193 Bellaterra, Spain
[2]ICREA–Institució Catalana de Recerca i Estudis Avançats, Pg. Lluis Companys, 23, 08010 Barcelona, Spain

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Flexoelectricity, describing the polarization response to a gradient of the strain, is a universal property of all insulators that has attracted considerable attention in the past few years. [1] In spite of its fundamental and practical interest, it has long resisted theoretical attempts at quantifying it with predictive accuracy in realistic materials. In this talk, I will introduce the methodological advances that have recently lifted this limitation in the context of first-principles electronic-structure theory. [2] I will discuss applications to perovskite-structure SrTiO3, either in the cubic [3] or ferroelastic tetragonal phase. [4] I will also emphasize the generality of these newly established theoretical tools, with interesting connections to the physics of orbital magnetism, natural optical activity and magnetoelectric couplings.

[1] M. Stengel and D. Vanderbilt, in "Flexoelectricity in Solids From Theory to Applications", edited by A. K. Tagantsev and P. V. Yudin (World Scientific Publishing Co., Singapore, 2016).
[2] Miquel Royo and Massimiliano Stengel, Phys. Rev. X 9, 021050 (2019)
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Nonlinear optics from first-principles real-time approaches

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In the past decades, many-body approaches based on the GW approximation and the Bethe-Salpeter equation have become the state-of-the-art for calculating optical absorption in solids and nanostructures. In this talk, I'll first present a real-time approach derived from the non-equilibrium Green's function, that allows to extend the GW+BSE approach beyond the linear regime.[1,2] Using this approach, I'll address the importance of many-body effects and in particular of excitonic effects for nonlinear optical properties.[3] For example, I'll look at the case of single-layer monochalcogenide whose strong Second Harmonic Generation cannot be reproduced within the independent- particle approximation.[4] In the second part of the talk, I'll then discuss the possibility of a real-time approach based on time-dependent density-functional theory, that can describe excitonic effects.[5]

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The Computational 2D Materials Database: High throughput screening for topological and ferromagnetic 2D materials

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We introduce the Computational 2D Materials Database (C2DB) [1], which presently contains 3712 (hypothetical) 2D materials. The database is publicly available and comprises a unique playground for investigating a wide range 2D materials properties. Here we first present an automated search for 2D insulators with non-trivial band topology, which resulted in 48 quantum spin Hall insulators, 7 Chern insulators and 21 crystalline topological insulators [2]. Roughly 75% are predicted to be dynamically stable and one-third was known prior to the screening. Finally we will discuss conditions for magnetic order in 2D (circumventing the Mermin-Wagner theorem) [3] and present 12 novel 2D insulators that are predicted to exhibit ferromagnetic order at *finite* temperatures [4].

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Electronic structure of two-dimensional antiferromagnetic transition-metal phosphorus trisulfides

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Since the separation of graphene, two-dimensional (2D) materials have been extensively investigated. Recently, magnetic 2D materials have emerged as an important subject. Based on previous neutron scattering spectroscopy and susceptibility measurement experiments, bulk van der Waals materials FePS3, NiPS3, and MnPS3 have been described by Ising-type, XY-type, and Heisenberg-type spin models, respectively. According to the so-called Mermin-Wagner theorem, however, the magnetization in two-dimensional systems is stabilized in Ising-type but not in XY- or Heisenberg-type systems. Moreover, the two-dimensional systems described by XY-type spin Hamiltonian hosts the so-called Kosterlitz-Thouless transition. In this presentation, I will introduce recent experimental results on the magnetic ordering of these three compounds from bulk to monolayers and explain how first-principles density-functional theory calculations can qualitatively and even quantitatively explain the experimental results.

[1] J.-U. Lee et al., "Ising-Type Magnetic Ordering in Atomically Thin FePS3," Nano Lett. 16, 7433 (2016).

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[3] K. Kim et al., "Suppression of Magnetic Ordering in XXZ-type antiferromagnetic monolayer NiPS3," Nat. Commun. 10, 345 (2019).

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Phonon-limited transport in 2D materials

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Recently, some of us identified close to 2000 exfoliable 2D materials from first-principles calculations [1]. We are now characterizing the scattering of electrons by phonons in this database, with the objective of finding electrostatically-doped 2D semiconductors with superior intrinsic transport properties.

This work relies on three developments : i) density functional perturbation theory to compute electron-phonon interactions with a truncated Coulomb interaction in the non-periodic direction and gates to induce doping [2]; ii) a high-accuracy and automated workflow to compute phonon-limited mobilities [3] by first identifying the electrons and phonons needed to describe the relevant scattering events and then solving the Boltzmann transport equation; iii) a more approximate workflow to estimate transport performances by selecting a small number of phonons (~ 10) which capture the main characteristics of electron-phonon scattering over the Fermi surface.

The approximate workflow scans hundreds of materials and screens outstanding new candidates. The high-accuracy workflow is then used on selected materials (~50). Several novel high-conductivity 2D materials are found. The data also provides valuable insights on electron-phonon scattering in 2D. Three aspects stand out: intervalley scattering, doping, and band anisotropy. We discuss their impact on transport, and how they can be exploited to find or engineer 2D semiconductors with high conductivities.

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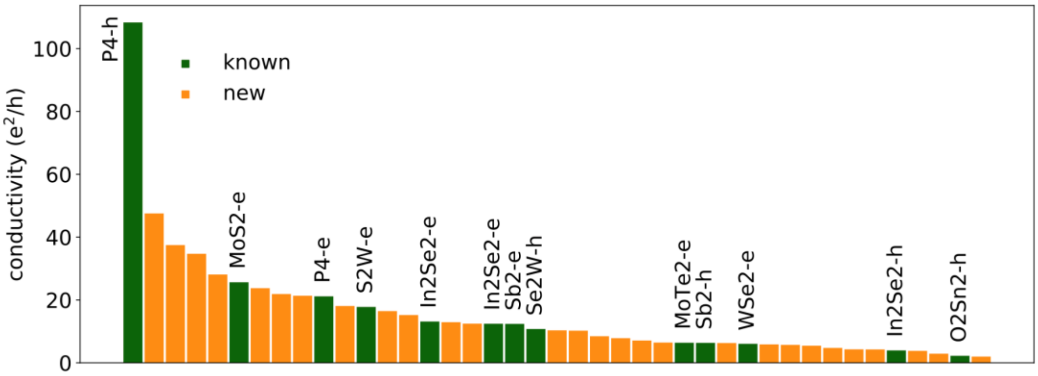

Figure 1: Phonon-limited conductivities of some 2D materials in our database, computed with a high- accuracy workflow [2]. Materials shown here were selected by screening a subset of smaller structures in our database. Already, several high-conductivity candidates were found.

Thursday January 9

TBA

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Ab-Initio Solution of the Many-Electron Schrödinger Equation with Deep Neural Networks

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Given access to accurate solutions of the many-electron Schrödinger equation, nearly all chemistry could be derived from first principles. Exact wavefunctions of interesting chemical systems are out of reach because they are NP-hard to compute in general [1], but approximations can be found using polynomially-scaling algorithms. The key challenge for many of these algorithms is the choice of wavefunction Ansatz, which must trade off between efficiency and accuracy. Neural networks have shown impressive power as accurate practical function approximators [2-3] and promise as a compact wavefunction Ansatz for spin systems [4], but problems in electronic structure require wavefunctions that obey Fermi-Dirac statistics. Here we introduce a novel deep learning architecture, the Fermionic Neural Network, as a powerful wavefunction Ansatz for many-electron systems. The Fermionic Neural Network is able to achieve accuracy beyond other variational Monte Carlo trial wavefunctions on a variety of atoms and small molecules. Using no data other than atomic positions and charges, we predict the dissociation curves of the nitrogen molecule and hydrogen chain, two challenging strongly-correlated systems, to significantly higher accuracy than the coupled cluster method, widely considered the gold standard for quantum chemistry. This demonstrates that deep neural networks can outperform existing ab-initio quantum chemistry methods, opening the possibility of accurate direct optimisation of wavefunctions for previously intractable molecules and solids.

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Singling Out Dynamic and Nondynamic Correlation

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The correlation part of the pair density is separated into two components, one of them being predominant at short electronic ranges and the other at long ranges. The analysis of the intracular part of these components furnishes a natural partition of the Coulomb hole and it permits to classify molecular systems according to the prevailing correlation: dynamic or nondynamic [1]. The study of the long-range asymptotics reveals the key component of the pair density that is responsible for the description of London dispersion forces and a universal decay with the interelectronic distance [2]. The application of these results to a two-electron two-atom model gives rise to indices of dynamic and nondynamic correlation based on natural orbital occupancies [3], which can be easily extended to provide a local picture of dynamic and nondynamic correlation [4]. The natural range-separation, the identification of the dispersion forces, and the kind of predominant correlation type that arise from this analysis are expected to be important assets in the development of new electronic structure methods in wave function, density, and reduced density-matrix functional theories.

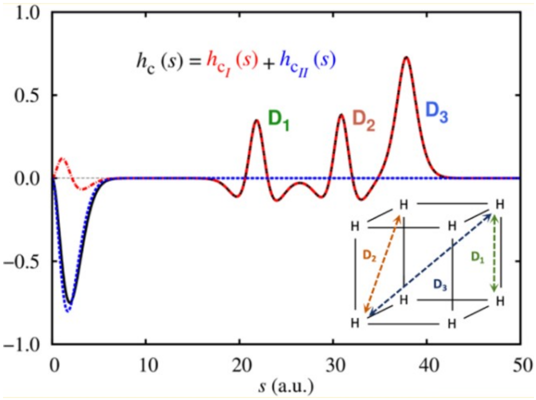

Figure 1: Separation of the Coulomb hole into short-ranged (blue) and long-range (red) parts for a cube of hydrogens.

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Strain effects in Fe-based superconductors: Nematicity, exotic magnetism and superelasticity

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In this talk we will analyze the role of strain in some families of Fe-based superconductors.
Via a combination of first principles-based calculations and many-body approaches we investigate nematicity, possible exotic magnetism and superelasticity in 122 and 1144 systems [1,2] and discuss possible origins of the discrepancy between ARPES measurements and electronic structure calculations in the nematic phase of FeSe [3] with the help of strain.

This work is a collaboration with Vladislav Borisov, Paul Canfield, Seok-Woo Lee, Rafael Fernandes, Peter Hirschfeld and Brian Andersen

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[2] Song et al. APL Mater. **7**, 061104 (2019)
[3] Zantout et al. (in preparation)

Low-valence layered nickelates: a cuprate analog for high-temperature superconductivity?

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The physics behind high-temperature superconductivity in cuprates remains a defining problem in Condensed Matter Physics. Among the multiple approaches to addressing this problem has been the study of alternative transition metal oxides with similar structures and electron count, proxies for cuprate physics. After 30 years of trying, a non-cuprate compound with a cuprate-like structure that exhibits superconductivity at high temperature has been found: hole-doped NdNiO2. Given that this material is a member of a series of layered nickelates, this result suggests the possibility of a novel family of unconventional superconductors. By means of first-principles calculations, we analyze the similarities and differences between this family of low-valence planar nickelates and cuprates. Even though these nickel oxide materials possess a combination of traits that are widely considered as crucial ingredients for superconductivity in cuprates (a square-planar nature, combined with the appropriate 3d-electron count, and a large orbital polarization) they also exhibit some important differences (a much larger d-p energy splitting, and lack of magnetism in the parent compound). Our results show that low-valence layered nickelates offer a new way of interrogating the cuprate phase diagram and are singularly promising candidates for unconventional superconductivity.

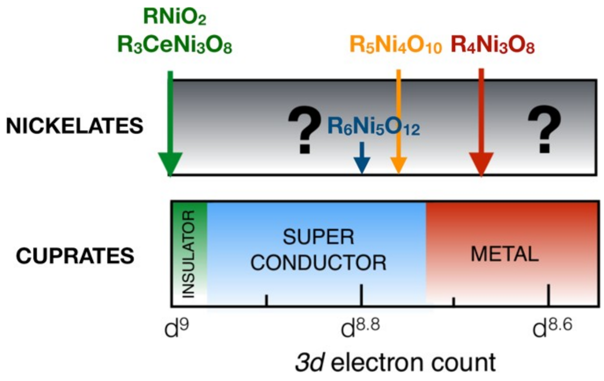

Fig. 1. Schematic phase diagram of layered nickelates (top) and cuprates (bottom) presented as a function of the nominal 3d electron count. R represents a Rare-Earth ion. For nickelates, only a few line compositions are known in the range of 3d electron count shown.

A topological tour through momentum space in memory of Alexey Soluyanov

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The aim of this talk is to give an overview tour of features in band structures that can be characterized by topological quantities such as fluxes or monopole charges. The basic representative of such a feature is a Weyl node degeneracy of two bands. I will highlight the distinction in two universal classes of type-I and type-II Weyl nodes and the ensuing physical consequences [1]. I will then continue to symmetry-protected features, including Dirac nodes, Nexus fermions and nodal lines. For each case, the symmetries protecting the band structure feature will be emphasized and material examples provided. A particularly intriguing case are be the nodal lines connected by non-symmorphic symmetries, so-called nodal chains [2]. Capitalizing on recent developments, I will close by discussing differences between the case of Hermitian systems with real energy eigenvalues and non-Hermitian, i.e., complex band structures. Examples for the latter will be given in the realm of metamaterials and topolectrical circuits, but can also be motivated by the eigenvalue structure of single particle Greens functions, for instance.

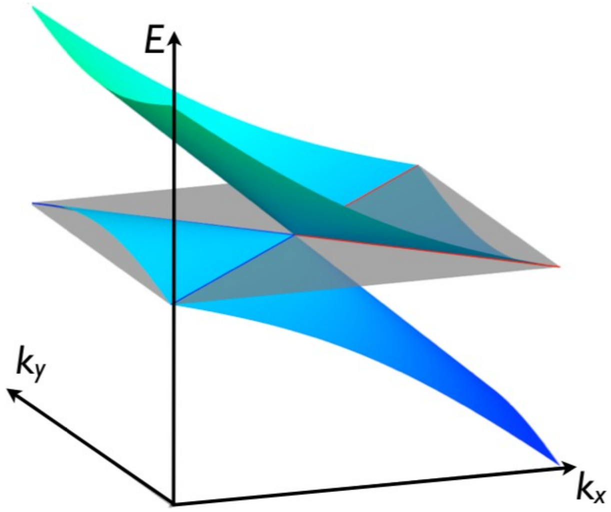

Figure 1: A type-II Weyl fermion (from [1]).

[1] A. A. Soluyanov *et al.*, Nature **527**, 495–498 (2015).
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Insights from magnetic Weyl semimetals: the Berry phase and beyond

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It is known that Bloch electrons pick up an anomalous velocity because of the Berry curvature in the magnetic material. Recent discovery of magnetic Weyl semimetals (WSMs) provides a novel, ideal platform to examine the Berry curvature-induced transport phenomena, such as the anomalous Hall effect (AHE) and the thermal version of AHE. In the AHE, we focus on the Wideman-Franz law that governs the fundamental correlation between the charge and heat transport. We reveal a novel mechanism [1] to violate the Wideman-Franz law at the finite temperature by the Berry curvature distribution rather than the inelastic scattering effect, which is distinct from the ordinary (longitudinal) transport. Beyond the linear-response phenomena like AHE, WSMs can generate giant nonlinear optical response (such as the DC photocurrent), which is commonly attributed to the Berry curvature too. As a WSM turns magnetic, however, we find a new class of photocurrent by re-examining the nonlinear response theory [2,3]. It is contributed by the diabatic effect, instead of the Berry phase. Because this is a leading-order phenomena, the induced photocurrent is expected to be much larger compared to the non- magnetic case.

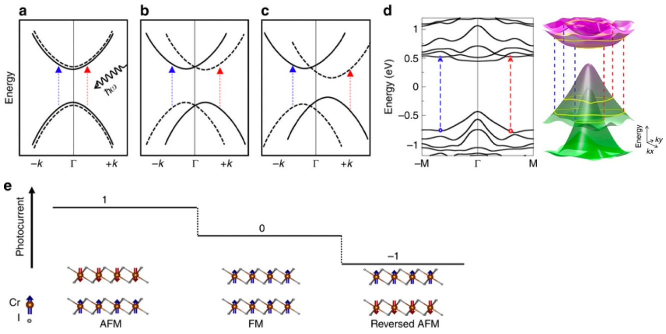

Figure 1: Band structure symmetry-breaking and magnetic structures of the bilayer CrI3. Schematics of band structures (a) with both inversion symmetry (P) and the time-reversal symmetry (T), (b) with only T but P-breaking, and c with both P- and T-breaking. For both (a), (b), the light excitation (ħω) at +k and −k is symmetric to each other. However, such a symmetry is broken in (c). As a consequence, excited electrons at +k and −k do not cancel each other in velocity, giving rise to a dc photocurrent. (d) The band structure of AFM bilayer CrI3. Here both P and T are broken as the case of (c), violating the k to −k symmetry. (e) The AFM, FM and reversed AFM phases display three distinct responses to a linearly polarized light – positive current state(1), zero current state (0) and negative current state(−1).

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Comprehensive search for topological materials using symmetry indicators

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Abstract [1,2] Topological materials (TMs) showcase intriguing physical properties defying expectations based on conventional materials, and hold promise for the development of devices with new functionalities. While several theoretically proposed TMs have been experimentally confirmed, extensive experimental exploration of topological properties as well as applications in realistic devices have been held back due to the lack of excellent TMs in which interference from trivial Fermi surface states is minimized. We tackle this problem in the present work by applying our recently developed method of symmetry indicators to all non-magnetic compounds in the 230 space groups. An exhaustive database search reveals thousands of TM candidates. Of these, we highlight the excellent TMs, the 258 topological insulators and 165 topological crystalline insulators which have either noticeable full band gap or a considerable direct gap together with small trivial Fermi pockets. We also give a list of 489 topological semimetals with the band crossing points located near the Fermi level. All predictions obtained through standard generalized gradient approximation (GGA) calculations were cross-checked with the modified Becke-Johnson (MBJ) potential calculations, appropriate for narrow gap materials. With the electronic and optical behavior around the Fermi level dominated by the topologically non-trivial bands, these newly found TMs candidates open wide possibilities for realizing the promise of TMs in next-generation electronic devices.

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Twistronics: Electron localization in stacked layers of 2D materials

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The stacking of individual layers of two-dimensional materials can be experimentally controlled with remarkable precision on the order of a tenth of a degree. Simple theoretical models, as well as accurate electronic structure calculations predict that the electronic properties in stacked 2D layers depend sensitively on the relative orientation (the “twist angle”) between successive layers; the term “twistronics” was introduced to describe this effect. For special twist-angle values, electron localization and high density of states can be achieved. We explore this effect in graphene, a semi-metal, and representative materials of the transition metal dichalcogenide family of semiconductors. This effect has important consequences for electronic behavior, including highly-correlated states and superconductivity, as has been recently reported for twisted bilayer graphene. We explore the conditions for and consequences of electron localization and the ensuing emergence of correlated sates in twisted bi- and multi-layer structures.

Towards Ferroics in 2-Dimensions

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Inspired by the global thrust towards miniaturization and by the ubiquitous research in two-dimensional (2D) materials, the talk will focus on the modelling of ferroelectrics and ferromagnets towards the 2D limit. In particular, I will pay particular attention to spin-orbit coupling (SOC), a relatively small interaction which however gives rise to a rich phenomenology in ferroics, ranging from Rashba effects in ferroelectrics to complex spin textures in exotic magnets. Within this framework, I will concentrate on the interplay between spin and dipolar degrees of freedom, by addressing layered ferroelectrics where SOC leads to a tight link between Rashba spin-splitting in the electronic structure, spin-texture and electric polarization. When time permits, I will also focus on the role of spin-orbit coupling in the magnetic properties of layered Nickel halides. In closer detail, the anisotropic exchange (often neglected in the literature) turns out to be relevant, when describing the magnetism of 2D-iodides, emphasizing the importance of relativistic effects related to the non- magnetic anion.

Friday January 10

Quantum electrodynamical density functional theory: First principle approach to cavity QED

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In this talk I present Quantum Electrodynamical (Time Dependent) Density Functional Theory (QED-DFT) – a recently proposed *ab initio* approach to the theory of atomic, molecular, and condensed matter systems strongly interacting with quantum electromagnetic field. I start from a general physical picture and a formal statement of the many-body problem for non-relativistic electrons strongly coupled to photon modes of a microcavity. Then I sketch the proof of basic QED-DFT mapping theorems and discuss possible approximation strategies. In particular I will introduce generalization of the concept of optimized effective potential that makes a connection of QED-DFT to many-body perturbation theory. Finally, I will discuss first applications of this approach and its connection to the theory of quantum dissipative systems.

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[3] M. Ruggenthaler, J. Flick, C. Pellegrini, H. Appel, I.V. Tokatly, A Rubio, Phys. Rev. A **90**, 012508 (2014)
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Current induced forces and removing periodicity in DFT+NEGF calculations

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We are trying to understand how systems under non-equilibrium conditions may be understood. The passing of high currents can be found in highly conductive nanostructures but constrictions limits the current. Recent studies show how nanostructured graphene can exhibit transistor like properties under non-equilibrium [1]. Here we use recent advances in DFT+NEGF methods to understand and examine the current induced forces in nanostructured graphene and C60 systems [2, 3]. We will present how bond charges and bond forces are correlated.
Together with current induced forces we also try to eliminate the necessary periodicity in DFT+NEGF calculations [4, 5]. We will present how one can easily, and with increased throughput, perform more accurate calculations by using real-space self-energies that represents infinite electrodes in multiple directions. Such electrodes leverages image couplings and improves electronic structure descriptions of e.g. long-range defects such as nitrogen defects in graphene.

[1] Zhang, H. et al. Nano Letters, **12**, 1772-1775 (2012); Sadeghi, H. et al PNAS, **112**, 2658 (2015); Sarwat, S. G. et al. Nano Letters, **17**, 3688-3693 (2017).
[2] Leitherer, S. et al. Physical Review B, **100**, 035416 (2019)
[3] Brand, J. et al. Nano Letters, **19**, 11 7845-7851 (2019)
[4] Papior et al, Physical Review B, **100**, 195417 (2019)
[5] Papior et al, Computer Physics Communication, **212**, 8-24 (2017)

Spin currents in collinear and non-collinear antiferromagnets

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Spin currents are one of the key concepts of spintronics. In the past, two types of spin currents have been predominantly discussed and utilized: the spin-polarized current in ferromagnetic materials and the spin Hall effect. The two spin currents are very different. The spin-polarized current only exist in magnetic materials, has a non-relativistic origin and flows in the same direction as the charge current. In contrast, the spin Hall effect exists also in non-magnetic materials, has typically a relativistic origin and is transverse to the charge current. In recent years it has been discovered, however, that the phenomenology of spin currents is much richer, and more types of spin currents can occur. We have shown that the spin-polarized current can also exist in some antiferromagnetic materials and that a new type of spin Hall effect exists, which has origin in the magnetic order, and occurs in ferromagnetic and some antiferromagnetic materials [1]. This effect is now referred to as the magnetic spin Hall effect and has been recently experimentally demonstrated in non-collinear antiferromagnet Mn_3Sn [2]. Furthermore, we have shown that the conventional spin Hall effect can exist in some non-collinear magnetic systems even in absence of the relativistic spin-orbit interaction [3]. Here we review the various types of spin currents that can occur in magnetic systems and give general conditions for their existence as well as a symmetry classification. In addition, we present calculations of these novel spin currents in various collinear and non-collinear antiferromagnets.

[1] J. Železný et al.: Phys. Rev. Lett. 119, 187204 (2017)
[2] M. Kimata et al., Nature 565, 627–630 (2019)
[3] Y. Zhang et al: New J. Phys. 20 (2018)

Simulating biosensors using a combination of non-equilibrium Green’s functions and QM/MM methods

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alexandre.reily@unesp.br

Solvated systems apear in a number of applications, from electrochemistry to biosensors. From a theoretical simulations point of view these are complex system from a number of aspects. In particular the design of all electronic biosensors requires that the device be imersed in – a typically aqueous – solution that involves a large configurational space. Furtheremore, biomolecules comprise large complex structures that are not always feasible with state of the art ab initio simulations. Finally, in an electronic biosensor, electrons must obviously be accounted for, hindering the use of fully classical molecular dynamics methods.

In this talk I will address a methology that finds a balance. Known as QM/MM, we combine it with a non-equilibrium Green’s function formalism to simulate electronic transport in graphene, graphene nanopores and nanogaps as possible platforms for DNA chips, and *de novo* sequencing. I will address the effects of the solvent on the electronic transport properties of such devices, and how the potential of water molecules, and particularly of charged counter ions completely alter the properties compared to simulations in the “gas phase”, and even open new channels for transport.

Exchange-correlation functionals for the band gap of solids

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I will first discuss the results of a recent benchmark study in which we evaluate the quality of exchange-correlation functionals for the determination of electronic band gaps of solids [1]. We compiled for this benchmark a dataset with information on the experimental structure and band gaps of 472 non-magnetic materials. This dataset was used to test around 50 functionals, ranging from standard local and semi-local functionals, passing through meta-generalized-gradient approximations, and some hybrids. I will then consider the two best functionals for band structures, namely the screened hybrid functional HSE06 [2] and the modified Becke-Johnson (MBJ) [3] exchange-correlation potential, and I will propose how to modify them to calculate accurate band alignments and defect energy levels at interfaces. This leads to a local hybrid functional for interfaces [4], extending the results of a previously developed density-dependent mixing for bulk crystals [5]. Unfortunately, hybrid functional calculations can still be challenging for large supercells containing interfaces. The MBJ exchange-correlation potential would be in that case the ideal choice, but it can be used only for bulk crystals. We turned therefore the coefficient *c*, that multiplies the Becke-Russel exchange potential, into a local function of the position, along the lines of what we had already done for the mixing paramater of hybrid functionals. Both local functionals yield results of comparable quality as GW at a significantly reduced cost. This is because we account properly for the position dependence of electronic screening, through a density estimator of the local dielectric function.

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Posters

P1

GW study of pressure-induced topological insulator transition in group IV-tellurides

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The electronic structure of group IV-tellurides presents a number of interesting characteristics. Notable among them is the fact that the electronic structure of all these materials seat close to a crossover between trivial and non-trivial topology [1]. In particular, SnTe is a topological insulator [2,3] characterized by an inversion of the symmetry of the states forming the top of the valence and bottom of conduction bands with respect to the trivial insulators PbTe and GeTe. The topological transition with composition has been observed in alloys [4] and the transition with pressure in PbTe has been proposed [5]. Here we use GW calculations to study the transition, as a function of volume and pressure, between a trivial and a non-trivial electronic structure topology for PbTe, SnTe and GeTe. We show that G_0W_0 introduces a significant correction on the values of the critical pressure with respect to ones obtained with density functional theory (DFT), and in the case of PbTe it even corrects the sign of the transition pressure. We also observe that near the transition, where G_0W_0 corrections may invert the order of the DFT bands, we need to go beyond the usual diagonal G_0W_0 approximation and include off-diagonal terms in order to avoid artifacts in the band dispersion near the band gap edges.

	PbTe	SnTe	GeTe
GGA	-2.5	-2.7	3.0
G_0W_0	4.8	-3.2	1.9

Table 1: Topological transition pressures in GPa calculated with GGA and G_0W_0.

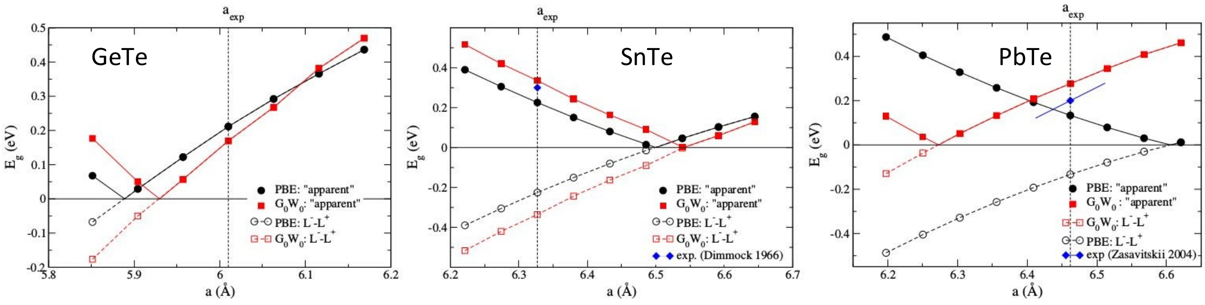

Figure 1: Band gap as a function of lattice parameter for GeTe, SnTe and PbTe. Solid lines: apparent band gap (lowest unoccupied state minus highest occupied state) at L. Dashed lines: band gap calculated as the energy difference between L^-_6–L^+_6 states. Experimental values are shown as diamonds. For PbTe we also display the experimental $\partial E_g/\partial V$.

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P2

Towards phase diagram of IrTe2 from first principles

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$IrTe_2$ adopts 1T structure with triple Te-Ir-Te layers at high temperatures, but below 220 K some Ir-Ir bonds shrink by over 20%, resulting in a modulated state with rows of dimers in a triangular lattice and a wave vector (1/5,0,1/5). At lower temperatures, various patterns of dimers are seen. We use first-principles calculations to parametrize a simplified model, that allows us to characterize the energetics and thermodynamics of dimerized phases, and compute the phase diagram of the system in the temperature-pressure plane.

P3

Self-consistent site-dependent DFT+U(+V) for defects

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DFT calculations of defects in transition metal oxides often require advanced methods such as hybrid functionals to yield a reasonable description of the electronic structure. When properties of defects at dilute concentrations are desired, the-often incompatible-need for large supercells is added to the above functional requirement. We have recently established self-consistent, site-dependent DFT+U and DFT+U+V as promising approaches to address the challenge of simultaneously meeting these requirements. The minimal added cost of DFT+U(+V) compared to a semi-local functional enables the treatment of large supercells, yet the structural and electronic properties relevant for point-defect calculations agree well with hybrid-functionals. We ascribe this to both the self-consistent determination of the Hubbard parameters that leads to an internal consistency of results, as well as the site dependence, which for localized defect states captures chemical changes on multivalent ions around the defect. We will highlight the performance of the method for oxygen vacancies in the perovskite oxides SrTiO$_3$ and SrMnO$_3$ [1]. In the former self-consistent DFT+U+V leads to an electronic structure of oxygen vacancies that agrees well with that of hybrid functionals, which also translates to similar formation energies that agree well with experiment. Moreover, the DFT+U+V results are much less dependent on the cell size compared to DFT or DFT+U (see Figure 1). In SrMnO$_3$ the site dependence of Hubbard U significantly lowers defect formation energies and the critical epitaxial strain for magnetic phase transitions.

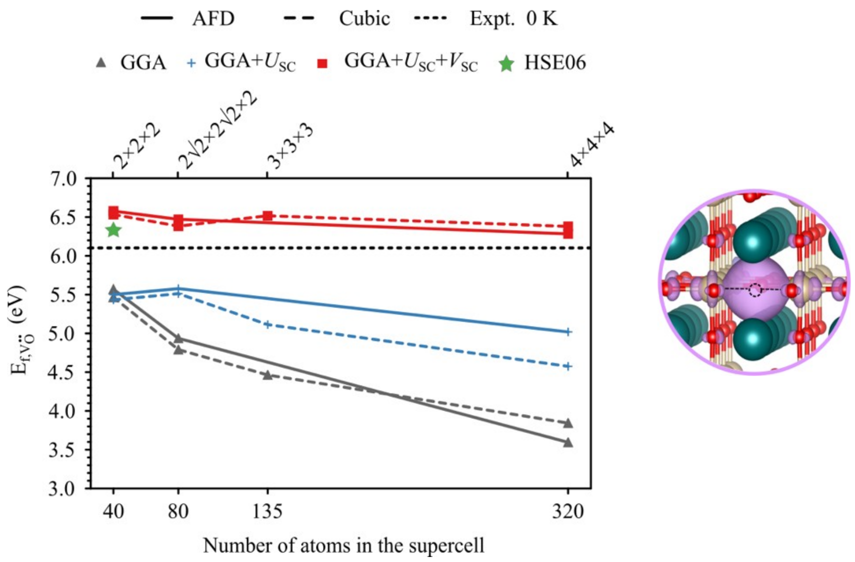

Figure 1: Oxygen vacancy formation energies in SrTiO$_3$ as a function of the supercell size and using different computational setups.

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P4

Anharmonic renormalization of flexural acoustic modes in graphene

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The mechanical stability and long-range crystalline order of two dimensional (2D) materials has always been under debate [1,2], however, since the discovery of graphene, the debate is only theoretical. 2D materials are invariant upon any rotation by putting the axis in the plane where the system is. This symmetry obliges the harmonic dispersion of the acoustic out-of-plane modes to be quadratic close to the point gamma in the first Brillouin zone, instead of linear, and this functionality makes the membrane unstable. The instability is translated as diverging atomic displacements as a function of the sample size and finite line width of phonons with very low crystal momentum[3,4].

These instabilities arise within the harmonic approximation, however, an anharmonic approach may suppress them. In this work we apply an anharmonic method, including quantum effects at a non-perturbative level, named SSCHA (stochastic self-consistent harmonic approximation)[5,6]. We see that the inclusion of anharmonic effects suppresses the divergence in the atomic displacements and provides a vanishing line width to the phonons with very low crystal momentum.

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P5

Towards a faster and simpler PAW Method

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Large scale electronic structure calculations require modern HPC resources and, as important, mature HPC applications that can make efficient use of those. Real-space grid-based applications of Density Functional Theory using the Projector Augmented Wave method [1] can give the same accuracy as DFT codes relying on a plane wave basis set but exhibit an improved scalability on distributed memory machines. The projection operations of the PAW Hamiltonian are found to be the performance critical part due to their limitation by the available memory bandwidth. We investigate on the usability of a 3D factorizable basis of Hermite functions (c.f. Figure 1) for the atomic PAW projector functions that allows to reduce and nearly to remove the bandwidth requirements for the grid representation of the projector functions in projection operations. This increases the fraction of exploitable floating-point operations on modern vectorized many-core architectures, like GPUs, by raising the arithmetic intensity of such operations [2].

With analytically given PAW projector functions the generation scheme for partial waves exhibits less tunable parameters and needs to be inverted compared to the traditional approach. As a test bulk properties and their convergence rates computed with the modified PAW data sets are reported.

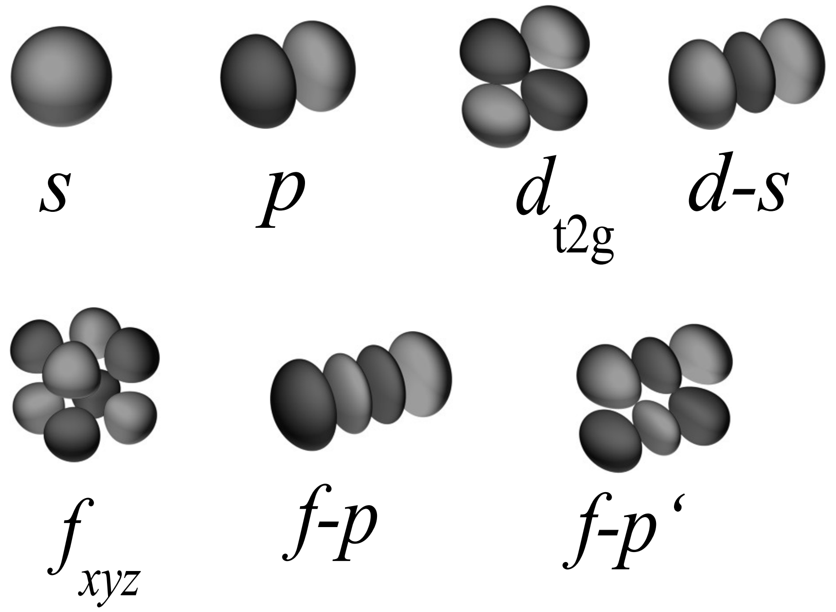

Figure 1: Spherical Harmonic Oscillator eigenstates are Cartesian products of 1D-functions. This property is exploited to increase the performance of projection operations by lowering bandwidth requirements.

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P6

Quantum Anharmonic Effects on the Superconducting LaH_{10}

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The discovery of superconductivity in the H_3S at 203 K revived the attention on superconductors described through the Bardeen-Cooper-Schrieffer (BCS) and the Migdal-Eliashberg theories. Furthermore, the constant advancing of experimental and computational tools for the investigation and prediction of the system properties significantly widened the landscape on superconductivity in the BCS hydrides.

One of the most recent breakthrough is the discovery of the Lanthanum hydride (LaH_x) with a record superconductivity temperature of 250 K at a pressure of 170 GPa [1], [2]. The multiple experimental studies performed for this system reported different and distant values for its superconductive temperature (T_c) [1], [2], [3]. This suggests the existence of multiple superconductive phases coexisting at the same pressure. This feature sums up to the not yet well known stoichiometry of the material.

In this study we apply first-principle calculations including anharminic effects within the Stochastic Self Consistent Harmonic Approximation [4] (SSCHA) in order to accurately characterize the supeconductive properties of LaH_{10}. Our results suggest that the crystal structure of LaH_{10} is stabilized by quantum nature of the ions. This is similar to the situation in H_3S [5]. The superconducting properties and T_c are consequently strongly affected by large anharmonicity. Our results in LaH_{10} point again that quantum anharmonic effects are crucial in high-temperature superconducting hydrides.

Acknowledgments: We have received funding from the European Research Council (ERC) under the European Unions Horizon 2020 research and innovation programme (grant agreement No 802533)

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P7

Electrical tuning of vibrational modes in Transition Metal Dichalcogenides

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We investigated the atomic scale tribological properties of transition metal dichalcogenides (TMDs) by using ab-initio techniques. Such compounds are formed by triatomic layers presenting MX2 stoichiometry (M: transition metal cation, X: chalcogen anion) held together by van der Waals forces.

We considered 6 various prototypes MX2 TMDs (M=Mo, W; X=S, Se, Te) with hexagonal P63/mmc symmetry, focusing on how some specific phonon modes contribute to their intrinsic friction.
Within the DFT framework, we described the exchange-correlation interaction energy by means of the PBE functional, including long range dispersion interactions in the Grimme formulation (DFT-D3 van der Waals).

We identified and disentangled the electro-structural features that determine the intra- and inter- layer motions affecting the intrinsic friction by means of electro-structural descriptors such as orbital polarization, bond covalency and cophonicity [1]. The study of the structural distortion modes allowed us to predict possible paths of exfoliations.

We show how the phonon modes affecting the intrinsic friction can be adjusted by means of an external electrostatic field. In this way, the electric field act as a knob to control the intrinsic friction.

The presented outcomes are a step forward in the development of layer exfoliation and manipulation methods, which are fundamental for the production of TMD-based optoelectronical devices and nanoelectromechanical systems.

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P8

Competition Between Structural and Electronic Phase Transitions in Perovskite Thin Films

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Perovskite materials exhibit a variety of intersting effects such as ferromagnetism, ferroelectricity, multiferroicity and superconductivity. In 2004[1], it was discovered that, under the right conditions, a two-dimensional electron gas (2DEG) could appear at the interface between polar and nonpolar perovskites such as LaAlO3/SrTiO3 (LAO/STO) as a response to the polar discontinuity there. This 2DEG can also display interesting properties such as magnetism and/or superconductivity. A phenomenological theory suggests that the appearance of the 2DEG with thin film thickness or an applied electric field across the film is continuous[2]. This theory does not consider competition with other effects such as the rotation of oxygen octahedral cages (tilts), which both LAO and STO can exhibit.

We have proposed a theory of 2DEG formation at a polar-nonpolar interface which includes coupling to tilts. We found that the tilts can change the nature of the appearance of the 2DEG in two ways: it can change the thickness or electric field required for the 2DEG to appear, and it can also change the transition from continuous to discontinuous (see Fig. 1). Understanding the role of the tilts could lead to an improved understanding and control over the appearance of the 2DEG. We will also discuss our first-principles calculations to further investigate and verify this theory.

One suggested method to improve control of the 2DEG is to replace the polar material with a ferroelectric material such as PbTiO3 (PTO)[3], so it could be easily switched on and off with an electric field across the film. In practice however, ferroelectric materials can already screen polar disconinuities by forming domain structures. Previous studies have suggested that there is competition between ferroelectric domains and 2DEG formation which depends on the thickness of the material[3]. However, evidence of 2DEG formation in polydomain ferroelectrics has recently been observed[4]. We have developed a model which addresses and explains coexistence between the 2DEG at ferroelectric domains. The ultrathin and thick limits agree with the previous competition-based study, but the two regimes are separated by a region where both effects are observed simultaneously.

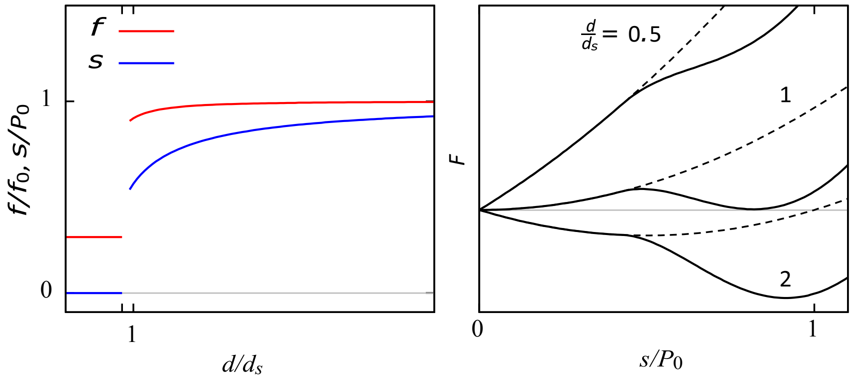

FIG. 1. A first order appearance of a 2DEG upon coupling to tilts. Left: the tilt angle f in units of equilibrium tilt angle f_0 and 2DEG carrier concentration s in units of polar discontinuity P_0 as a function of film thickness. d_s is the critical thickness obtained from the uncoupled

theory. Right: energy curves F of the coupled theory as a function of carrier concentration for various film thicknesses. The dashed lines show the corresponding energy curves of the uncoupled theory at the same thicknesses.

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P9

Quantum enhancement of charge density wave in NbS_2 in the 2D limit

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At ambient pressure, bulk 2H-NbS_2 displays no charge density wave instability at odds with the isostructural and isoelectronic compounds 2H-$NbSe_2$, 2H-TaS_2 and 2H-$TaSe_2$, and in disagreement with harmonic calculations. Contradictory experimental results have been reported in supported single layers, as 1H-NbS_2 on Au(111) does not display a charge density wave, while 1H-NbS_2 on 6H-SiC(0001) endures a 3×3 reconstruction [1,2]. Here, by carrying out quantum anharmonic calculations from first-principles, we evaluate the temperature dependence of phonon spectra in NbS_2 bulk and single layer as afunction of pressure/strain. For bulk 2H-NbS_2, we find excellent agreement with inelastic X-ray spectra and demonstrate the removal of charge ordering due to anharmonicity. In the 2D limit, we find an enhanced tendency toward charge density wave order. Freestanding 1H-NbS_2 undergoes a 3×3 reconstruction, in agreement with data on 6H- SiC(0001) supported samples. Moreover, as strains smaller than 0.5% in the lattice parameter are enough to completely remove the 3×3 superstructure, deposition of 1H-NbS_2 on flexible substrates or a small charge transfer via field-effect could lead to devices with dynamical switching on/off of charge order [3].

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P10

Electronic Transport in $Mo_2ScC_2O_2$ MXene

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With the advancement of experimental technologies and theories, the outstanding properties of MXene materials have been widely investigated [1]. The low-dimensional d-metal carbides or nitrides have been suggested to possess good electrical properties when the MXene elemental composition and/or their surface terminations are appropriately designed [2]. However, the investigations on the potential applications of MXenes in electronic devices are still in the starting stage up to now [3]. The electronic transport properties of conductive MXene have been found to be strongly influenced by surface terminations[4], therefore it would be important to investigate the pure MXene with different surface functionalize elements.
In this work, we chose to study O-functionalized Mo_2ScC_2 MXene using first-principles calculations. The electronic transport properties for model devices made out of $Mo_2ScC_2O_2$ MXene are investigated using nonequilibrium Green's functions and the current–voltage characteristics are predicted. We hope that our findings may provide new clues for the design of practical nano-electronic devices of MXenes.

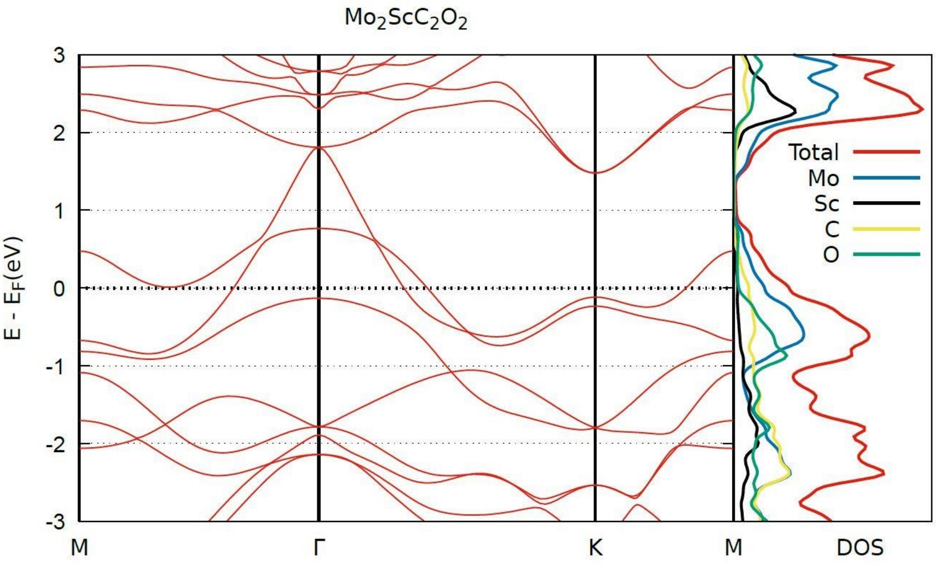

Figure 1: Band Structure and Density of States for $Mo_2ScC_2O_2$

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P11

Theoretical study in DFT of bi-metallic compounds of transition metals with cyclic ligand

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Bimetallic complexes represent a unique class of compounds that have attracted considerable attention, and in particular, concerning the electronic interaction between metal centers **[1]**. The most obvious and impressive feature is their mixed valence that allows charge transfer between metal centers **[2]**.

These delocalized derivatives are of great interest because of their potential applications in the development of new organometallic materials with ferromagnetic and / or optical properties **[3, 4]**. In recent years, we have developed a research area dedicated to the study of monometallic hetero-polycyclic complexes in which a ring is π-bonded to the L3M fragment (L3 = (CO) 3, Cp-) **[5]**. According to previous studies, bi-nuclear systems have proven to be very selective catalysts compared to mononuclear species. As a result, we extended our theoretical study to binuclear transition metal complexes with aromatic hetero-polycyclic nitrogen ligands.

A common feature of bimetallic complexes is the presence of direct metal-to-metal bonds where electronic communication between two metal centers can change the particular chemical and physical properties of the metal complexes. As is known, this communication depends on the binding with the ligands and the nature of the metal centers. The magnetic, optical and redox properties of this type of complex depend on the strength of the electronic interactions between the metal centers.

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P12

Deciphering the electronic structure of 5-armchair graphene nanoribbons and its topological end-states

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5-armchair graphene nanoribbons (5-AGNRs) are the narrowest from the 3 p+2 family, with p an integer, which are predicted to have the smallest band gaps compared to the other AGNR families [1]. They have been already successfully synthesized with atomic precision, for instance via on-surface synthesis methods [2, 3]. Nevertheless the electronic structure measurements show a substantial discrepancy, with reported band gap ranging from 0.1 eV up to 2.8 eV. Here we performed an extensive characterization of the electronic structure of 5-AGNRs by combining scanning tunneling microscope (STM) and spectroscope (STS) measurements, recorded on both Au(111) substrate and decoupling NaCl layer, with density functional theory (DFT) calculations. We demonstrated the presence of in-gap ”end”-states at the termini of finite ribbons that become degenerate and single occupied after reaching a certain ribbon length, explaining the apparent disagreement on the assignment of the band gap on previous studies. We show that these end- states are topological in nature and that they have magnetic character, both theoretically and via STM-tip lifting experiments.

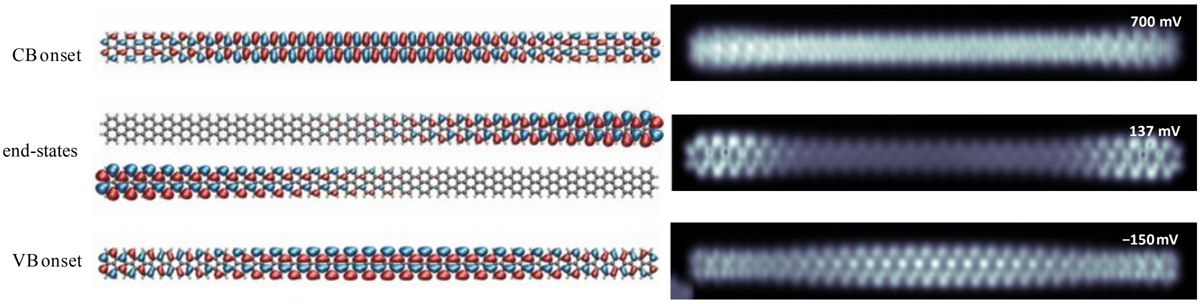

Figure: (left) DFT-calculated 30 unit-cell long 5-AGNR molecular orbitals corresponding to the valence band (VB) and conduction band (CB) onsets and in-gap end-states; (right) Measured constant height dI/dV images (scale bar 1nm).

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P13

Structural and electronic properties of puckered-buckled arsenene lateral heterostructures

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Since the discovery of the two-dimensional (2D) materials such as graphene [1], silicene [2], germanene [3] phosphorene, etc., with unique optical, electrical, mechanical, transport and gas sensing properties, the interest in studying these 2D systems has increased significantly. Searching for new alternatives, two stable allotropes of arsenic have been found, with honeycomb-like atomic structure and thickness of one monolayer of arsenic, similar to black and blue phosphorene. These two allotropes of arsenic present a puckered and buckled honeycomb structure, however both of them are indirect gap semiconductor with a gap of the order of 0.8 eV [4] and 1.6 eV [5], respectively. These two allotropes display different electronic properties. Because of the rapidly advance in crystal growth techniques and the synthesis of different structures, materials and compounds, the idea of synthesizing lateral heterostructures appears to be one of the attractive systems to investigate. Different investigations have demonstrated the enhanced performance of the heterojunctions or lateral heterostructures when compare with single structures. For example, diodes and photodiodes based on WSe_2-WS_2 junctions have been shown to display excellent rectification behavior and large photocurrent generation [6]. Black-blue phosphorene heterostructures exhibit metallic and semiconductor features depending on the interface formed by them [7]. It is important to study arsenene lateral heterostructures because it shows promising electronic and transport properties features. In this work, the density functional theory (DFT) is applied as implemented in the computational code SIESTA to investigate the structural stability, density of states and band structures of the arsenene lateral heterostructures.

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P14

Multiscale modeling of radiation effects on biological matter and functional materials for missions to Mars

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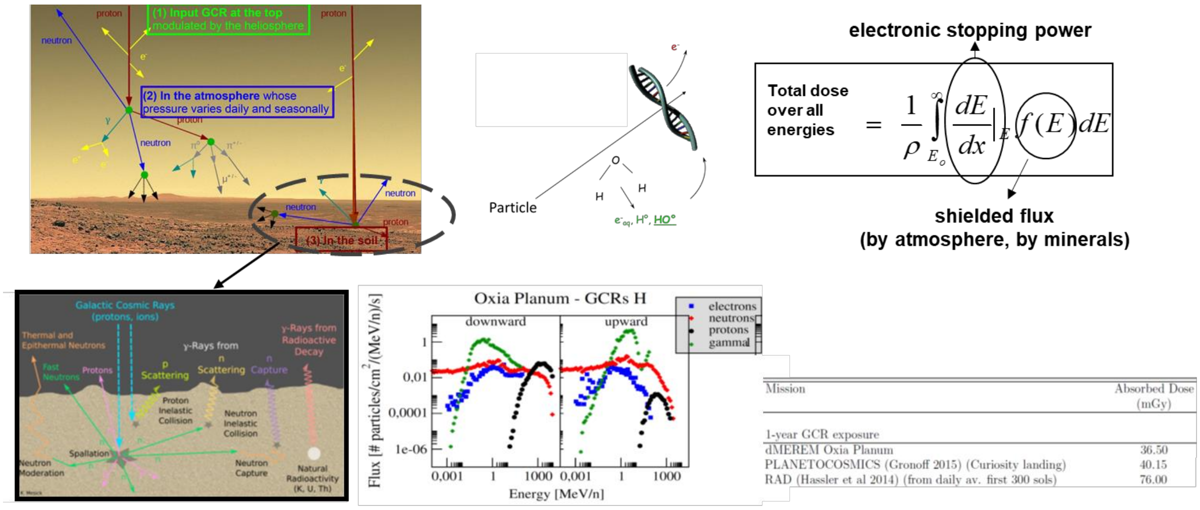
The modeling of space radiation (mainly protons and electrons) effects on spacecraft materials and/or biological molecules as proxies for astronauts is of high importance for planning future missions to deep Space and to other planets. As Mars lacks a dense atmosphere and a magnetic field (that would both protect from the radiation coming from the Sun and from galactic cosmic rays), future explorers on the planet and the overall infrastructure and devices they carry will be strongly affected by radiation.

The study of radiation effects in matter implies a multiscale modelling approach [1]. First stage effects can be studied via Monte Carlo particle transport, as implemented for example in Geant4 [2]. Here we have performed a study, with Geant4, on the overall radiation environment at locations of interest for the coming missions and on the first-stage induced effects in the human body, expressed here by the doses, linked to the *electronic stopping power* in water, as a function of the incoming radiation and of the capability of certain minerals to shield radiation (Fig.1).

There are some limitations in the study of radiation effects as generally done via the sole Monte Carlo particle transport approaches. In particular, Geant4, commonly used for planetary studies, has no accurate treatments of effects near particle stopping (low speed), for example the linear response treatment of the electronic stopping is used illegally in a wide energy range, there is no synergy between electronic and nuclear stopping, all targets are considered as amorphous. More importantly, in the biological context, Geant4, even more than Geant4-DNA [3], has a relatively limited description of low energy electrons, loosely defined as those with kinetic energy below ~1–10 keV, which actually mostly contribute to energy deposition at the nanoscale, associated with important subcellular structures (e.g., DNA).

The results show fair agreement with previous modelling studies [4] but underestimation with respect to measurements from the NASA Curiosity rover at Gale Crater [5], highlight that risk limits for human health established by NASA as support for a 1-year and a 30-day stay on the planet are not overpassed and show some potential of locations where hematite is more abundant to lower the doses on water.

The work sets the stage for developing a multiscale approach for radiation effects on both biological targets and functional materials of use for future space and planetary missions *(see poster by B. Gu and by N. Koval)* .



$$\text{Total dose over all energies} = \frac{1}{\rho}\int_{E_o}^{\infty}\left(\frac{dE}{dx}\right|_E f(E)\,dE$$

Mission	Absorbed Dose (mGy)
1-year GCR exposure	
dMEREM Oxia Planum	36.50
PLANETOCOSMICS (Gronoff 2015) (Curiosity landing)	40.15
RAD (Hassler et al 2014) (from daily av. first 300 sols)	76.00

Figure 1: The radiation environment at the surface of Mars is given by both the downward particle shower generated in the atmosphere by Galactic Cosmic Rays (GCR) and the backscattered radiation from the minerals in the surface and subsurface. Water is the main component of biological matter, and doses in water are calculated to estimate the radiation effects in human explorers. Both the radiation environment (particle spectra) and doses at Oxia Planum on Mars (landing site of the next ESA's mission) are calculated via Geant4, the state of the art Monte Carlo particle transport code used in simulation of planetary environments..

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P15

Band gap modulation of dynamically stable bilayer and trilayer WS_2 configurations under external electric field

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Effective modulation of the band gap of two dimensional layered materials via external electric field is a tantalizing possibility that would bring two dimensional materials based electronics one step closure [1]. Among the various intriguing two dimensional materials, WS_2 is one of the emerging classes of 2D materials with fascinating properties and is formed by stacking of atomic layers of S–W–S in a sandwich configuration [2]. As we move beyond the monolayer WS_2 structure, the different stacking possibilities of the S–W–S atomic layers leave us with multiple configurations; among them the dynamically stable ones can be interpreted via phonon dispersion calculation. In this work, by means of density functional theory based calculations, we systematically examined the stable formations of differently stacked bilayer and trilayer WS_2 structures including the effect of Van der Waals interaction and further studied the variation in their band structures by application of external electric field.

We found two dynamically stable configurations for bilayer WS_2 with no imaginary frequencies in their phonon dispersion and five such configurations for trilayer WS_2 and named them as AA', AB and AA'A, AA'B, ABA, ABA', ABB' respectively according to their stacking and orientations. Within the generalized gradient approximation, the bilayer WS_2 structures were found to be indirect band gap materials with band gap values 1.34 and 1.33 eV respectively. The trilayer WS_2 configurations also revealed indirect band gap with values 1.13, 1.17, 1.19, 1.16 and 1.17 eV respectively. Although the valance band maximum for all the configurations (both bi and trilayers) was universally located at the Γ point within the k-space, the position of CBM shifted in between Γ and K point for AA'A, AA'B and ABB' configurations whereas the same for all other configurations were found to be situated at the K point. Next we applied external electric field in the normal direction to the layer by including the effect of the crucial monopole and dipole correction in the calculation. Band gaps of both the bilayer WS_2 configurations were observed to be decreasing sharply with the increasing strength of the external electric field and both of them eventually became metallic at field strength of value 2.6 V/ nm. Notably, the band gap became direct at the K point for field strength of 1.9 V/ nm and 1.5 V/ nm respectively for AA' and AB configurations. The asymmetry in the stacking of AB configuration seemed to have hardly any effect on the variation of band gap as electric field decreased almost symmetrically for electric field along opposite directions. Although the band gap also decreases continuously with increasing field strength with similar indirect to direct transitions, the scenario is quite different for trilayer configurations as the rate of decrement in the band gap is much slower and metallic nature has been achieved at field strength as high as 11 to 12 V/ nm. Also the stacking asymmetry have notable effect on the band gap variation as the metallic nature was achieved at different values of the field strength for electric field along opposite directions for AA'B, ABA' and ABB' configurations. We attribute the nature of variation in the bandstructure to the symmetry breakdown between the S–W–S layers with increasing field strength which localizes the HOMO and LUMO at different layers and to the change in diffusivity of the p_z orbital associated with the S atom. The diffusive nature of the p_z orbital of S atoms increase for both bi and trilayers with increasing field strength but the localization of the HOMO and LUMO are more symmetric for the bilayer configurations compared to the trilayers. We further interpreted our results in terms of giant stark effect and obtained a robust relationship. In light of our findings, it would appear that dynamically stable bilayer and trilayer WS_2 configurations could significantly expand the known space of layered materials with widely tunable band gaps and provide further avenues for novel nanoelectronics and photonics application.

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P16

Band Gap of 3D Metal Oxides and Quasi-2D Materials from Hybrid Density Functional Theory

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The problem of describing the Kohn-Sham (KS) band gap in materials with insulating and semiconducting character is well-known in the solid-state physics and chemistry research domain. On the computational side, two major issues arises during the comparison of the KS band gap from semilocal GGA (generalized gradient approximation) calculations with experimental data, primarily exclusion of the excitonic effect, and the secondly presence of standard approximations in density functional theory. The topic is one of the long standing problems in this researcher community, and debated in various first-principles based computational research articles. On the experimental aspect, this crucial information of the band gap can be obtained from different experimental techniques. For example, the well adopted method of the optical absorption spectra in the UV-VIS region of the light source or determination of the band-edges position from the direct or indirect photo-emission spectroscopic measurements.

The failure of the semilocal DFT (density functional theory) functionals is partially revisited from the hybrid functionals or the version from self-consistent dielectric-dependent (DD) functionals. In this work we have partially touched this band gap issue by reinvestigating (see Fig. 1) 24 bulk oxides (3D) and 24 quasi two-dimensional (2D) materials from global hybrid (B3LYP, PBE0), short (SC-BLYP, HSE06) and long range-separated (CAM-B3LYP) hybrid functional and their DD version (DD-B3LPY, DD-SC-BLYP, DD-CAM-B3LYP) [1]. The conclusions of the work further corroborated with the principal component analysis (PCA).

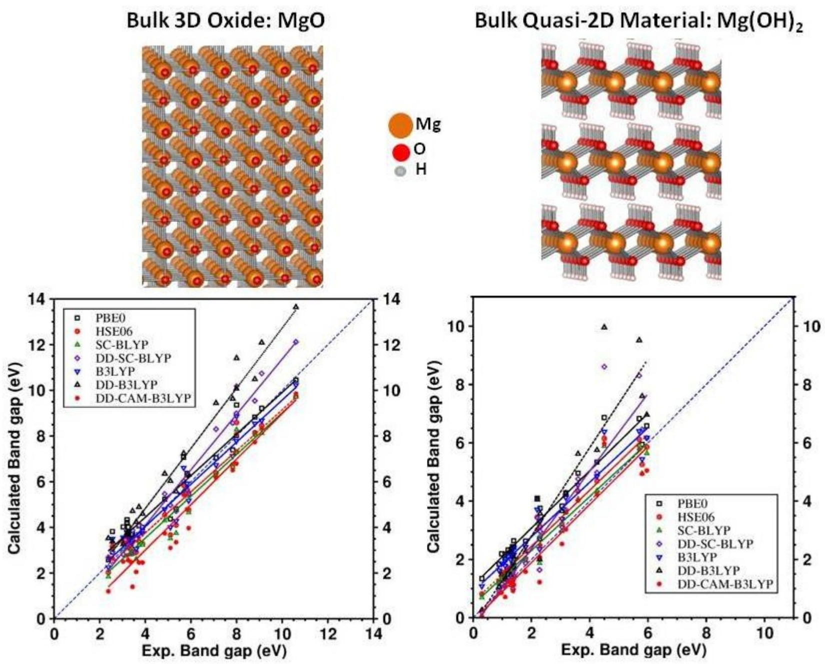

Figure 1: Calculated band gaps from various hybrid functional for 24 3D metal oxides (left panels), and 24 bulk quasi-2D materials (right side panels) from different hybrid functionals.

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P17

Electronic structure optimization of nanoporous graphene

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As an effort towards the expansion of graphene's fields of applications, a new 2D atomically precise holey material was synthesized in 2018: nanoporous graphene (NPG) [1]. This novel structure exhibits outstanding electronic properties, such as a semiconducting gap, highly directional transport and electronic states localized in the vacuum pore regions (pore states). These properties allow us to envision multiple potential applications in carbon nanocircuitry, sensing and sieving, which place nanoporous graphene as a state of the art multifunctional material. However, the electronic pore states lie too high in energy, so that the electronic structure needs to be modified in order to bring to life some of the proposed applications.

Aimed at tuning the pore states, in this work we explore different optimization strategies, such as Li adatom adsorption [2] and pore size/shape modifications. Using Density Functional Theory (DFT) we predict a downshift of the pore states and the appearance of nearly free electron (NFE)-like states that could lead to new quantum phenomena. Therefore, our results confirm both the efficacy of the considered tuning strategies and the strong versatility of nanoporous graphene.

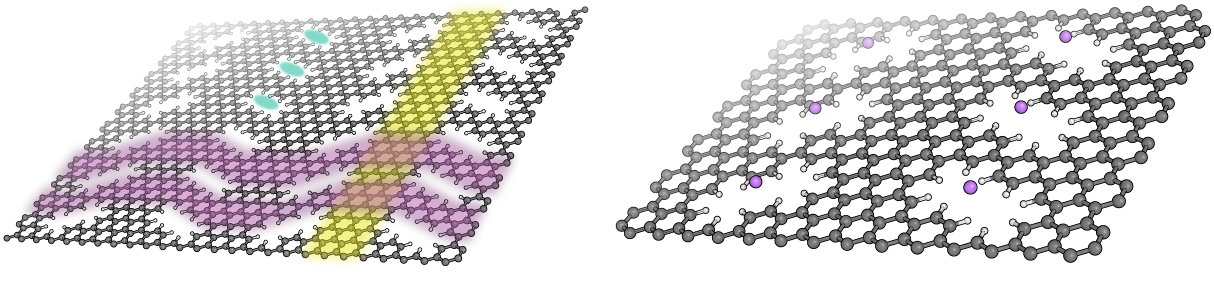

Figure 1: Different types of electronic bands in NPG (left) and Li decoration strategy (right).

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P18

Characterization and Stability of Janus TiXY (X/Y= S, Se, and Te) Monolayers

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The realization of Janus MoSSe monolayers has brought two-dimensional (2D), ternary transition metal dichalcogenides (TMDs) into focus. The addition of third element can lead to superior properties, hence extensive analyses on the characterization of these sophisticated systems are required to reveal their full potential. In this study, we examine the structural, mechanical, electronic, thermal, and optical properties of TiXY (X/Y= S, Se, and Te) monolayers by using first-principles techniques. In addition to the common 1T form, 2H phase is considered and the stability of both phases are revealed by phonon spectrum analysis and molecular dynamics simulations. Following the investigation of the mechanical response, electronic structures are examined together with partial density of states analysis. While monolayers of 1T-TiXY are found to be semimetals, monolayers of 2H-TiXY are semiconductors with indirect band gap. The optical spectrum is obtained by calculating the frequency dependent imaginary dielectric function and is correlated with the electronic structure. The variation of heat capacity with temperature is investigated and low/high temperature response is shown. Finally, possible structural distortions/transformations are also taken into account and charge density wave transition in 1T-TiSeS due to Peierls instability is demonstrated. Our results not only reveal the stable Janus monolayers of 2H- and 1T-TiXY but they also point out these systems as promising candidates for nanoscale applications. [1]

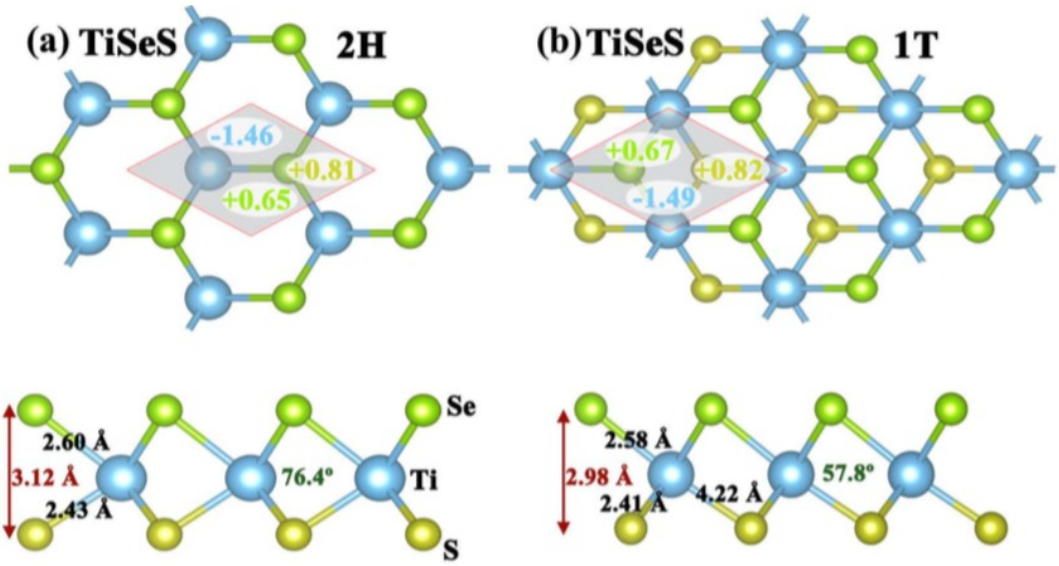

Figure 1: Top and side views of (a) 2H- and (b) 1T-TiXY systems.

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P19

Controlling type-II Dirac semimetal NiTe$_2$ electronic and elastic properties via strain and alkaline-element intercalation

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NiTe$_2$ crystallizes in a hexagonal structure with CdI$_2$ as prototype [1], as illustrated in Figure 1. The compound is an example of a Transition Metal Dicalcogenide (TMD), a class of quasi-2 dimensional materials of general composition MX$_2$ (M = transition metal and X = S, Se, or Te). TMDs have been extensively studied for decades for housing a huge variety of distinct physical phenomena and characteristics relevant to various applications, ranging from battery systems to nanophotonics devices and nanoelectronics [2]. Within this scope, electronic and elastic properties of the equilibrium, strained, and intercalated NiTe$_2$ were systematically studied within the scope of the Density Functional Theory (DFT). The compound shows tilted symmetry-protected Dirac-cone features derived from p-orbital bands near the Fermi level, characterizing a type-II Dirac semimetal. The analysis of the results suggest that single orbital-manifold band-inversion explain the mechanism behind the topologically non-trivial states. We have also shown that different applied strains are an effective route to perform the tuning of the trends of this bulk material. For instance, extension in the *z* direction is enough to promote Dirac fermions to the Fermi energy, lowering the overlap between the wave functions of low-energy valence-bands states, and suppress other usual non-relativistic bands from the Fermi surface. This can potentially bridge the way for non-conventional electronic devices, as alkaline-metal doping into the van der Waals gap of the structure can produce the desired strain without altering the electronic scenario.

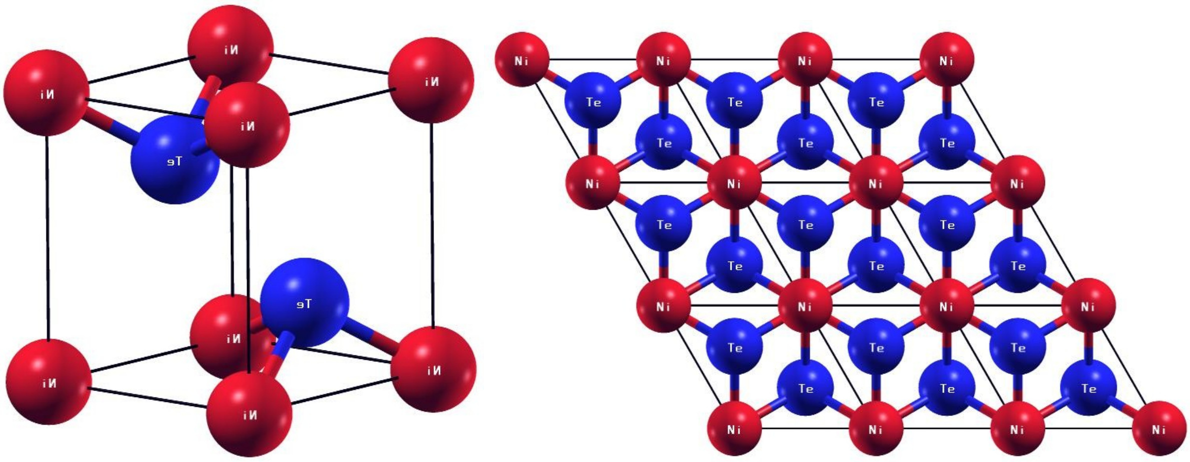

Figure 1: NiTe$_2$ unit cell and top view of several adjoining unit cells.

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P20

Electronic stopping power using Floquet theory: examples and applications.

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In a recent work [1] we showed how a general stationary theory for the electronic excitations in crystalline solids by a constant-velocity projectile can be defined based on Floquet theory for time-periodic systems [2]. When a projectile of radiation is shooting through a periodic crystalline potential defining a translational invariance in a space-time diagonal ($\boldsymbol{r} \rightarrow \boldsymbol{r} + na\boldsymbol{v}/|\boldsymbol{v}|$, $t \rightarrow t + n\tau$ with n integer, and $\tau = a/|\boldsymbol{v}|$), a transformation to the projectile reference frame makes the problem purely time-periodic with period τ. While the system is manifestly non-conservative in the 'laboratory' frame, it is quasi-energy conservative in the projectile's frame, which defines (stroboscopically) stationary solutions, determined within the framework of a single-particle Bloch-Floquet scattering theory. This represents a natural generalization of previous non-linear theories for the homogeneous electron gas [3].

The introduction of a joint density of states (JDOS) for the allowed electron transitions in model insulators provides interesting insights regarding the $v \rightarrow 0$ non-trivial adiabatic limit and the characterization of velocity thresholds in insulators. Furthermore, the emerging stationary solutions can also be considered as reference states for possible instabilities along the space-time symmetric direction, in analogy with charge density waves in space, or time-crystals in time: this could provide a theoretical justification for the 'flapping' instability recently investigated in TDDFT simulations [4]. The application of the formalism to simple idealized models already provides interesting insights and results, not easily accessible within previous frameworks. Moreover, the theory provides a new paradigm for the understanding of electronic stopping processes, and should lead to predictive computational schemes possibly more efficient than today's.

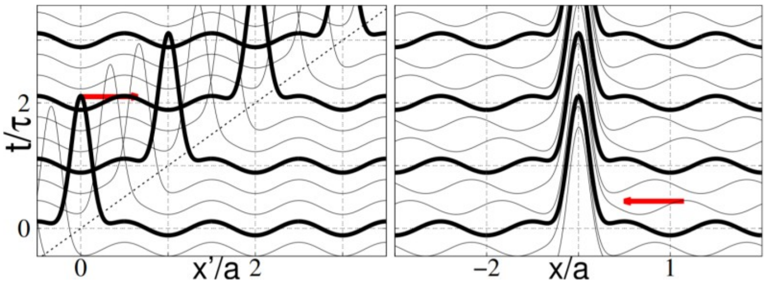

Figure 1: Evolution of the sum of a crystalline and a projectile potential in one dimension, both in the laboratory reference frame (left) and in the projectile's (right). The curves depict potential versus x, and are shifted for different times.

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P21

Ab-initio study of the electron-phonon interaction of a single Fe adatom on the MgO/Ag(100) surface

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Controlling the magnetic moment of individual atoms is a technologically important challenge due to potential applications in high density storage devices. Breakthrough experimental studies have recently shown that it is possible to create stable magnetic quantum states in individual adatoms [1– 3]. While the role of electronic interactions on the magnetic stability has been thoroughly investigated theoretically [4–6], the coupling with phonons has attracted much less attention.

The aim of this work is to study, via ab-initio calculations, the effect of the electron-phonon interaction (EPI) in Fe adatoms deposited on MgO/Ag(100), a benchmark system where the EPI is believed to determine to large extent its magnetic stability [3]. Here we present the calculated electronic structure and vibrational dynamics of this system, including the local vibrations of the adatom. Furthermore, we analyze the effect of the EPI on the magnetic stability via the renormalization of the electronic properties of the adatom.

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P22

Magnetic oscillations induced by phonons in non-magnetic materials

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An unexpected finding two decades ago demonstrated that Shockley electron states in noble metal surfaces are spin-polarized [1], forming a circulating spin texture in reciprocal space. The fundamental role played by the spin degree of freedom was then revealed, even for a non-magnetic system, whenever the spin-orbit coupling was present with some strength. Here we demonstrate that similarly to electrons in the presence of spin-orbit coupling, the propagating vibration modes are also accompanied by a well-defined magnetic oscillation even in non-magnetic materials. Although this effect is illustrated by considering a single layer of the WSe_2 dichalogenide, the phenomenon is completely general and valid for any non-magnetic material with spin-orbit coupling. The emerging phonon-induced magnetic oscillation acts as an additional effective flipping mechanism for the electron spin and its implications in the transport and scattering properties of the material are evident and profound.

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P23

Simulation protocols for paramagnetic transition-metal oxides

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Pauli paramagnetic crystals have an odd number of electrons in their crystallographic unit cell, but no long-ranged magnetic order. As such, they are necessarily degenerate metals, and certain transition-metal compounds among them are known to be poor metals or correlated-electron metals to varying degrees. Fully-oxidized transition-metal paramagnetic are of possible technological interest and are the focus of the present preliminary work, since they can exhibit almost elemental-metal-like electronic, thermal, and optical conductivities while remaining inherently resistant to oxidation. Particularly where they form in cubic or perovskite structures, they can simultaneously exhibit high elastic moduli, indentation hardnesses, and melting temperatures.

From a first-principles theory and simulation perspective, even supposedly weakly-correlated transition-metal oxide Pauli paramagnets are interesting from a number of perspectives. Firstly, since they have an half-integer number of electrons per unit cell per spin, but zero spin-polarization everywhere, it may be anticipated that they exhibit considerable many-body static correlation error in the total-energy within local, semi-local, and even hybrid functional approximations for exchange-correlation in (generalized Kohn-Sham) DFT. Secondly, since their partially-filled bands at the Fermi level are of d-electron character and hence relatively flat, with attendant strong Coulomb interactions, the scope for the non-recovery of accurate spectroscopic features such as effective masses and plasmon satellites (or Hubbard bands, depending on perspective) by the Kohn-Sham eigensystem is considerable (the paradigmatic system for this is $SrVO_3$ [1]). Lastly, these systems are never far from symmetry-breaking transitions, which are of intrinsic interest, and moreover of practical use as it has been recently shown that accurate crystallographic and spectroscopic properties can be calculated for oxides at half-filling by deliberately and randomly breaking available symmetries in approximate DFT applied to moderately large super-cells [2].

Here, we provide an overview of experimental findings on selected Pauli paramagnetic oxides and of work to date on simulating their properties. With a particular view to our own prediction of relatively advanced materials characteristics in these systems such as thermal conductivities, heat capacities, thermoelectric and plasmonic figures of merit, and the combination of these in multi-scale models for nanostructures, we explore in this poster which of the available theories (e.g. density or Green's function based), methods (including mean-field and multi-reference Hubbard U correction) and codes is most appropriate for this field of application.

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P24

3d transition metal oxide chains: spin-phases, magnetic exchange coupling and anisotropy

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Recently, the growth of 3d transition metal oxide chains with stoichiometry $Me\mathrm{O}_2$ (Me=Ni, Co, Fe, Mn) on Ir(100) and Pt(100) surfaces has been reported [1-3]. The competition between magnetic couplings along the chain and substrate-mediated interactions results in chiral non-collinear spin structures in some of those systems [2,3]. By means of density functional theory with Hubbard U corrections (DFT+U) we explore different magnetic properties of free standing $Me\mathrm{O}_2$ chains, see Figure 1a), aimed at understanding their relationship with the electronic band structure. First, considering different values of the correlation parameter, U-J=0, 1.5, 5 eV, we have obtained the spin-phase diagram as a function of the structural parameters. We find that large U values are needed to have stable high-spin phases, the highest being S=2 for FeO_2, see Figure 1b), and MnO_2. In the equilibrium configurations, we find that MnO_2 prefers a ferromagnetic (FM) ordering and that the other *Me* chains are antiferromagnetic (AFM). From the study of their band-structure, we conclude that the preference of an AFM (FM) configuration is associated to the insulating (conducting) character of the chain. The Ir(100) surface has the effect of filling up the partially filled MnO_2 bands, thus driving it to the experimentally found AFM state. We have also studied the magnetocrystalline anisotropy energy (MAE), by including spin-orbit interaction (SOI) in the DFT calculations. None of the studied systems has the easy magnetization axis along the chain. This property is contributed by the SOI at all the band crossings, e.g. in FeO_2 the magnetization is perpendicular to the chain, dominated by the crossing of bands with dz^2-up and dxz-up characters, see Figure 1c).

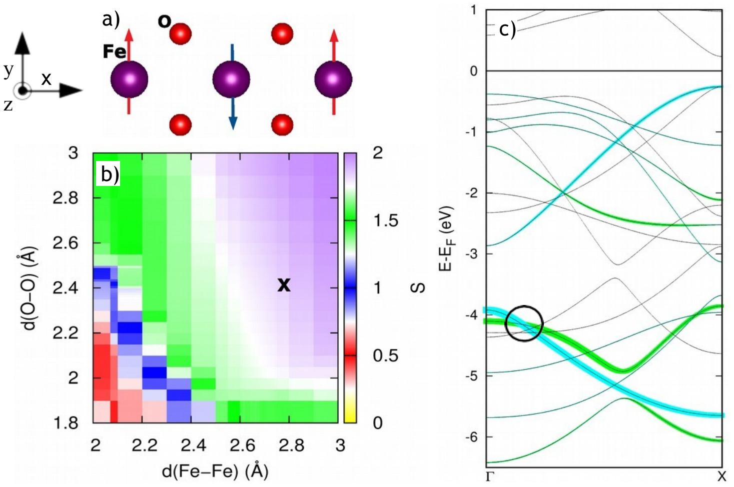

Figure 1: Sketch of the FeO_2 chain. a) Structure of the chain with AFM coupling. b) Spin-phase diagram with a correlation of U=5 eV. **x** shows the ground state configuration. c) Band-structure without SOI for U=1.5 eV. The circles indicates the main contribution to the MAE, colors indicate the orbital character of the band: blue is dxz and green is dz^2.

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P25

Electronic stopping power for protons in liquid water from TDDFT simulations with geometry pre-sampling

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Recent development of real-time time-dependent density functional theory (rt-TDDFT) methods enabled the calculation of electronic stopping power (S_e) for ions travelling through a target material, along a single trajectory. This approach has been successful for metallic systems in which the electronic density is relatively uniform is space[1]. However, for systems exhibiting less uniform densities, or disordered systems like liquids, it is still a challenge to obtain a meaningful S_e with a single or even a few trajectories, that can be compared to observations. The straightforward approaches of sampling trajectories on a uniform grid, or stochastically, require a relatively large number of trajectories for convergence, and hence they are computationally demanding[2]. To bridge the gap between the S_e derived from limited rt-TDDFT simulations and experimental data, we propose an ion trajectory pre-sampling method. This method selects trajectories on a geometric basis, by comparing the probability distribution function (PDF) of the distance between the projectile and the nearest atoms for the supercell to be simulated via rt-TDDFT, with the converged distribution obtained for a large sample. Trajectories are scored according to the overlap between sampled and converged distributions for all chemical species present in the target material, e.g. H and O in water. A convergence criterion for increasing number of trajectories is proposed and implemented. The S_e of liquid water for swift protons at the Bragg peak with v_{proton} = 1.72 a.u. is calculated via rt-TDDFT simulations at the PBE/6-311G** level, using the Gaussian and augmented plane wave method as implemented in CP2K[3,4]. The simulation box has dimensions of 24Å×16Å×16Å, and contains 203 H_2O molecules. The trajectories are 20Å-long, along the x-axis. As shown in Figure 1, the calculated S_e quickly converges to 1.63 a.u. – the generally used reference from the SRIM package[6], using only a handful pre-sampled paths. As a comparison, converging S_e to the same level of accuracy using uniformly distributed trajectories of the same length required at least 64 of these[6].

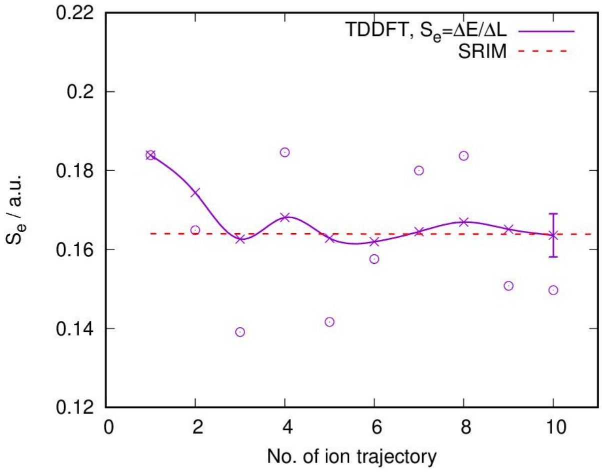

Figure 1: The purple line shows the convergence of the electronic stopping power (S_e) for protons in liquid water at the Bragg peak, corresponding to a velocity of v_{proton}=1.72 a.u. This is computed as a running average over 10 trajectories selected according to the PDF scoring criterion. Open circles show the S_e for each single trajectory. The dashed red line corresponds to the SRIM value.

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P26

Ab initio modeling of materials properties: an application to thermoelectric magnesium silicide alloys

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The need of clean and sustainable energy sources has driven an intense research effort in the field of material science. Besides abundant and recyclable, these materials must show rich transport properties to ensure their efficiency in energy conversion. By that means, here we present a detailed density functional theory (DFT) study of the electronic properties of magnesium silicide thermoelectric alloys. We discuss total energy calculations, electronic parameters, and the importance of the computed quantities in characterization methods, e.g., through Raman spectroscopy. These materials present interesting thermoelectric performance that we explain from our calculations.

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P27

Phonon Topology on the Buckled Honeycomb Lattice (An application of the methods of Topological Quantum Chemistry)

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We use methods of Topological Quantum Chemistry to analyze the topology of phonons on crystals with the structure of the buckled honeycomb. We show that there are a total of eleven gapped phases, nine of which turn out to be topological (five of them necessarily according to TQC). We also compute the most general dynamical matrix consistent with the system symmetries, including up to third nearest neighbour interactions. Computing the phonon bands of different compounds by DFT shows whether they are near a topological phase or not.

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Density functional perturbation theory with DFT+Uin the mixed-basis framework

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DFT+U is a viable tool to improve description of materials, where the standard DFT exchange-correlation potentials fail to catch essential properties of electronic correlation. While phenomenological in nature, it is numerically efficient and also gives access to energy derivatives, e.g. forces and force constants. Most applications to lattice dynamics properties have been based on the direct method (supercells and force calculations), while calculations utilizing the linear response approach have been rare [1,2].

Here I describe a combination of DFT+U and density functional perturbation theory (DFPT) in the framework of the mixed-basis approach, an efficient method based on norm-conserving pseudopotentials employing a combination of plane waves and tailored local functions for the expansion of the valence states [3]. The DFPT extension of the mixed-basis method [4,5] has been extensively applied in the past. The present DFT+U implementation employs the fully rotationally invariant form introduced in [6] in its relativistic extension [7]. It can be combined with calculations including spin-polarization or spin-orbit interaction. Its usefulness is demonstrated for compounds containing 3d or 4f/5felements.

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P29

Exchange-diffusion Monte Carlo

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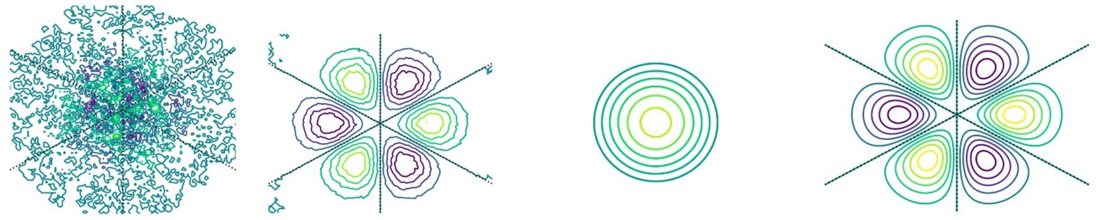
Quantum Monte Carlo (QMC) methods have provided some of the most important results in computational physics [1] and remain amongst the most accurate methods available for calculating ground state properties of quantum systems [2]. However, for certain systems, QMC suffers from the so-called *fermion sign problem*, the general solution to which has been shown to be an NP-hard problem [3]. We focus on *diffusion Monte Carlo* (DMC) as applied to electronic systems. Here, the sign problem arises when fermionic exchange symmetry forces the ground state to adopt a complex structure of regions where the wavefunction takes a particular sign, known as *nodal pockets*. The boundary between nodal pockets is known as the *nodal surface*.

The most popular approach to combat the sign problem in DMC is known as the *fixed- node approximation*, developed in the early 80s [4], whereby the nodal surface is fixed to that of some trial wavefunction, which must be known *a priori*. By treating the fermionic problem as a constrained stochastic optimization, we develop and implement an asymptotically exact formalism of fermionic DMC that makes no reference to a trial wavefunction. We demonstrate how this implementation informs alternatives to the fixed-node approximation and present some results for small atomic and molecular systems.



(a) DMC wavefunction with exchange moves, but without a stochastic nodal surface $\implies$ bosonic collapse.

(b) DMC wavefunction with exchange moves and a stochastic nodal surface.

(c) Analytic bosonic ground state (+ve definite).

(d) Analytic fermionic ground state.

Figure 1: Sample graphics.

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P30

Directional shift current and dipole selection rules in mirror-symmetric BC_2N

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We study the shift-current optical response in a noncentrosymmetric polytype of the quasi-2D layered semiconductor BC_2N [1]. Employing a recently developed first-principles Wannier-interpolation technique [2] implemented in the latest release of Wannier90 [3], we find that the photoconductivity exhibits two distinctive features at the band edge. First, it ranks among the largest bulk nonlinear responses reported to date, and peaks in an energy range suitable for optical manipulation. Secondly, it is strongly anisotropic, due to the vanishing of particular tensor components not foretold by phenomenological symmetry arguments; this is a consequence of dipole selection rules imposed by mirror symmetry, which imply that the relative parities between valence and conduction bands are key for determining the directionality of the band-edge response. The implications of the dipole selection rules should apply to a broad class of nonlinear responses.

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P31

Topological Semimetals with Butterfly-like Four-Point Intersecting Ellipses

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We introduce a particular type of semimetals, hosting eliptical nodal lines that cross giving rise to butterfly-shaped four-point intersecting ellipses (FPIE). In point-node semimetals, like Weyl [1] or Dirac [2] semimetals, valence and conduction bands cross in discrete points of the Brillouin Zone, while in the semimetals we introduce, two valence and two conduction bands are involved in crossins along closed paths in a plane of the Brillouin Zone. We identify the symmetry criteria for the existence of these nodal structures in time-reversal invariant spinless systems with negligible spin-orbit coupling. Particularly, we focus on the cases in which Kramers degeneracy plays an important role in the protection of the intersection between elipses. Following these symmetry criteria, we identify the space-groups that can host these exotic FPIEs and the possible centers for the elipses. Via DFT calculations, we propose ZrP_2 as candidate for hosting the introduced nodal structures.

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P32

Accurate methods for the description of binding energies of molecular solids

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The study of molecular solids has grown thanks to their significance as pharmaceuticals, organic semiconductor materials, and many other applications [1]. They can often have a rich phase diagram or exhibit polymorphism. Polymorphic lattice energy differences are typically very small, on the level of one per cent of the lattice energies [2]. Reliable theoretical prediction of the binding energies of molecular solids and their polymorphs requires accurate methods, which faithfully describe all the interactions between the particles. Many electronic structure techniques, including periodic density functional theory (DFT), periodic second-order Møller-Plesset perturbation theory (MP2), and diffusion Monte Carlo, have become an increasingly important tool for modeling molecular solids and polymorphism [3]. However, one issue of applying theoretical methods within periodic boundary conditions (PBC) for molecular solids is that there are several numerical parameters that affect the results, such as potentials, energy cutoff of the plane-wave basis set, and real space grid density. Therefore, it is necessary to obtain converged binding energies of molecular solids with respect to these numerical parameters if one wants to understand the accuracy of given theoretical methods. Converging with these parameters increases significantly the overall cost of the calculations. An alternative approach to obtain the binding energies of molecular solids is many-body expansion (MBE) which assembles the binding energy from contributions of 1-body, 2-body, 3-body and higher-order terms. Nevertheless, there are also some numerical parameters in this scheme, such as basis set, F12 setting, that need to be controlled to obtain converged binding energies of molecular solids. In this study, we calculate the lattice energies of some small-molecule solids with varying physicochemical properties by using PBC and MBE approaches with DFT, random phase approximation (RPA) and MP2 methods to clarify some of the issues related to both approaches. The binding energies of molecular solids obtained from different methods are then compared with experimental values to identify the trend in their accuracy.

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P33

TBFIT: An open-source software package for Slater-Koster tight-binding parameter fitting

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We introduce a newly developed open-source toolkit [1] for reliable fitting energy bands obtained from ab initio electronic structure calculations using two-center Slater-Koster tight-binding parameters [2]. The new toolkit has the genetic algorithm and the Levenberg-Marquadt nonlinear least square fitting algorithm to compute various hopping parameters between any given set of atoms. Moreover, advanced material parameters such as topological invariants can be computed readily using the Wannier charge center method. Using the code, we report a new tight-binding parameter set of bulk Bi crystals up to the sixth nearest neighbor hoppings which can be used for the thin film cases. We contrast two distinct parameter sets showing seemingly same electronic energy bands with different topological properties of bulk Bi. This highlights that the topological index or parameter needs to be treated carefully for proper parameterizations of first-principles energy bands of topological materials. The tight-binding model also reflects realistic Bi (111) surface in the sense that it faithfully reproduces the overall band structures of the surface obtained from first principle DFT calculations. For example, in a sharp contrast to the famous third-neighbor Liu-Allen model [3], our six-neighbor model does not suffer from mirror chirality mismatch issue on the surface band dispersion.

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P34

Electronic stopping power for protons in solar-cell materials from first-principles calculations

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Solar cells are used as a primary power source in spacecrafts and are continuously exposed to space radiation. Energetic protons, electrons, and ions interacting with solar cells can create atomic defects, which can reduce their performance. Thus, it is essential to study how these particles interact with the materials of solar cells. The key physical quantity that characterizes the impact of a particle onto a target is the so-called stopping power, denoted as $S(x) = dE(x)/dx$, which is the energy loss of a projectile, dE, per unit path length inside the target, dx. The energy of the impinging particle is dissipated into different degrees of freedom (electronic, nuclear, vibration), depending on the type and energy of the radiation and on the properties of the material it passes through.

In this work, we focus on the electronic stopping power (ESP), which is determined by electron-hole pair excitations, ionization, and collective charge (plasmon) excitations. We calculate ESP of Ge, GaAs, and Ga0.5In0.5P layers of the multilayer solar cells for the impact of protons using real-time time-dependent density functional theory and Ehrenfest dynamics as implemented in the SIESTA code [1, 2]. Previously, similar calculations of the electronic stopping power for Ge [2] and Ga0.5In0.5P [3] have been already done. Here we extend these studies and explore the effects relevant in the context of space applications. We consider different trajectories of a proton inside the target materials and impact kinetic energies in the keV range. We compare our results with the calculations in Refs. [2,3] as well as with the SRIM data [4].

We also characterize the radiation environment and effects (both the ionizing dose, linked to the ESP, and the non-ionizing dose, linked to atomic displacements) for exposure of solar cells during a possible Space mission scenario, via Geant4-based tools implemented in the SPENVIS interface (www.spenvis.oma.be).

Project funded by the Research Executive Agency under the European Union's Horizon 2020 Research and Innovation program (project ESC2RAD: www.esc2rad.eu, grant 776410).

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P35

Assessment of optimally-tuned range-separated hybrid functionals for the calculation of excited state properties in organic dyes

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Organic dye molecules are used in a wide variety of applications such as lasers, solar cells, and even as photocatalysts[1]. For all these applications, it is essential to understand the excited-state properties of the dye molecules. Currently, theoretical investigations of excited state properties usually employ time-dependent density functional theory (TD-DFT) or high-level wave-function based methods, such as the complete active space perturbation theory up to second order (CASPT2) or coupled cluster (CC) approaches. While TD-DFT based calculations are computationally very efficient, they often lack the accuracy of computationally more expensive wave-function methods[2]. However, the recently developed class of optimally-tuned range-separated hybrid (OT-RSH) functionals, which adjust parameters based on first-principles conditions, promise to at least reduce this gap in accuracy[3].

In this work, we assess the accuracy of OT-RSH functionals for excited-state properties obtained with TD-DFT, for organic dye molecules and precursors. Our findings focus on structural parameters (e.g., bond lengths, bond angles, etc.) as well as on energetic properties (e.g., vertical and adiabatic excitations) of the lowest-excited singlet states of these molecules. To test the accuracy of our results, we compare them to experimental findings and data from high accuracy wave-function methods from literature.

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Proximity and Defect Induced Band Gap Renormalization in 2D $PdSe_2$

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During the last decade, great efforts have been made to study two-dimensional transition metal dichalcogenides which belong to a special class of materials with a wide variety of technologically useful properties. Noble-metal dichalcogenides attract special attention due to their atomic and electronic properties. Recently, stable mono- and bilayer $PdSe_2$ with intriguing pentagonal morphology have been synthesized by exfoliation from its bulk crystal and using molecular beam epitaxy deposition on graphene surface [1,2]. However, the reported electronic properties could likely be influenced. For instance, the band gap of epitaxial bilayer $PdSe_2$ on the top of graphene and bigraphene should be decreased due to the proximity induced interlayer interaction whereas optical gaps of mechanically exfoliated $PdSe_2$ layers could likely affected by defects which normally occur during exfoliation and growth of monolayers.

Using combined density functional and accurate many body perturbation approaches at the GW-BSE level we quantitatively predict fundamental and optical gaps in 2D $PdSe_2$ and explain experimentally observed electronic properties resolving inconsistencies between experiment and theory. Including electron-hole interactions responsible for exciton formation, we solve the Bethe-Salpeter equation on top of the GW0 approximation to predict the optical properties. The calculated optical spectra of both mono- and bilayer $PdSe_2$ cover a wide region of solar flux demonstrating promising application in solar cells and detectors. These findings provide a basis for a deeper understanding of the physical properties of $PdSe_2$ and $PdSe_2$-based heterostructures.

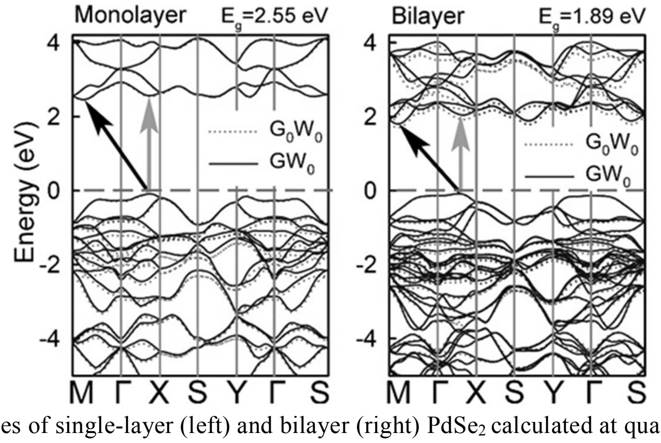

Figure 1: Band structures of single-layer (left) and bilayer (right) $PdSe_2$ calculated at quasiparticle G_0W_0 (dotted) and GW_0 (solid) levels. The indirect and direct band gaps denoted by black and grey arrows [3].

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[3] A. Kuklin *et al.* Phys. Rev. B **99** (24), 245114 (2019).

P37

Computational attempts to approach magnetism in metal-organic frameworks (MOFs)

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Metal Organic Frameworks (MOFs) attract attention because their magnetic properties can be tuned by changing the ligand moiety and the metallic centres [1]. Here, we focus our attention on two newly synthesised MOFs with linkers disposed accordingly to the *kagomé* tilling topology and coordinated by Cu or Co centres [2]. Despite the similar geometry, they show different electronic configurations and different magnetic behaviour. Density functional theory (DFT) calculations are used as an effective tool to improve our insight in the mechanisms that regulate their geometry-properties relationships.

The structural properties have been obtained employing the PBEsol exchange-correlation functional. However this method is known to poorly describe localized *d*-orbitals, hence the whole electronic structure. This usually results in an underestimation of the electronic band-gap. Traditionally such limitation is overcome including a Hubbard correction term (U), or relying on hybrid functional (e.g. HSE06). Surprisingly, we found that both schemes could not reproduce experimentally measured band-gap. Either because of technical computational limitations or because of the poor description of metals' states. We managed to obtain a proper description only introducing an unusual hybrid HSE06+U scheme [3-5]. However the agreement with the experiments is only qualitative and further efforts are needed in future to improve the results.

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P38

Control of spintronic properties of bimetallic MXenes via surface functionalization

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MXenes are two dimensional transition metal carbides (or nitrides) with the general formula M_2C (M = transitional metal). They are exfoliated from a corresponding parental phase with general formula $M_{n+1}AX_n$ (for simplicity MAX) by etching in aqueous hydrofluoric acid at room temperature [1-2]. Recently it has been shown that it is possible to synthesize more complex MAX phases with two metals centers, e.g. $(Mo_{2/3}Sc_{1/3})_2AlC$ and $(V_{2/3}Zr_{1/3})_2AlC$ [3-4] or metallic vacancies e.g. $(Mo_{2/3}\square_{1/3})_2C$ (□ = vacancy). Due to their synthesis MXenes are decorated by functional groups which type and distribution can be thermodynamically controlled. The tuning of such functional groups and stoichiometry can affect heavily the electronic band structures [5].

These systems are of particular interest because the interplay of stoichiometry and surface functions can lead to the formation of 2D half-semiconductor or half-metallic materials, a rare occurrence for 2D systems, which is fundamental to spintronic applications [6-7]. Therefore we screened several MXenes materials considering different metals, compositions, and functional groups. After testing, we identified $(V_{2/3}Zr_{1/3})_2CX_2$ (X = O,F and OH), $(V_{2/3}\square_{1/3})_2CF_2$ and $(V_{2/3}\square_{1/3})_2C(OH)_2$ as ideal materials. Among them, $(V_{2/3}Zr_{1/3})_2CO_2$ MXene is predicted to be an intrinsically ferromagnetic half-semiconductor with a remarkably high Curie temperature of 270 K. The results presented in this study establish a new family of MXenes with intrinsic magnetism, which makes them ideal candidates for spintronic applications in the near future.

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P39

A Comparative Study Using State-of-the-art Electronic Structure Theories on Solid Hydrogen Phases under High Pressures

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Identifying the atomic structure and properties of solid hydrogen under high pressures is a long-standing problem of high-pressure physics with far-reaching significance in planetary and materials science. Determining the pressure-temperature phase diagram of hydrogen is challenging for experiment and theory due to the extreme conditions and the required accuracy in the quantum mechanical treatment of the constituent electrons and nuclei, respectively. Here, we demonstrate explicitly that coupled cluster theory can serve as a computationally efficient theoretical tool to predict solid hydrogen phases with high accuracy. We present a first principles study of solid hydrogen phases at pressures ranging from 100 to 450 Gpa. The computed static lattice enthalpies are compared to state-of-the-art diffusion Monte Carlo[1,2] results and density functional theory[3] calculations. Our coupled cluster theory results[4] for the most stable phases including C2/c-24 and $P2_1/c$-24 are in good agreement with those obtained using diffusion Monte Carlo, with the exception of Cmca-4, which is predicted to be significantly less stable. We discuss the scope of the employed methods and how they can contribute as efficient and complementary theoretical tools to solve the long-standing puzzle of understanding solid hydrogen phases at high pressures. We also show that with recently developed techniques[5,6] in boosting the efficiency in CCSD, it will be possible to obtain forces and use them to optimize structures on the level of CCSD theory.

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P40

Strong multi-layer dependency of exothermic dissociation in polymeric nitrogene: Towards high energy density inorganic materials

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At ambient pressure and temperature, nitrogen exists as a triple-bonded dimer N_2 molecule in the gaseous form. The extreme strength of the triple bond is responsible for the inertness of nitrogen gas. However, single and double bonded allotropes of nitrogen give rise to the possible application of them as High Energy Density Materials (HEDM). The notion that other allotropes besides N_2 can be a source of a large amount of energy stems from the energy difference between single-bonded and triple-bonded nitrogen. On dissociating from a polymeric single-bonded structure (~ 40 Kcal mol^{-1}) to triple-bonded (~225 Kcal mol^{-1}) N_2, the amount of energy that is released can render nitrogen to be a strong contender as an HEDM [1–3]. These HEDMs will also prove to be environmentally friendly as the final product will be pure non-toxic nitrogen gas.

In this work, mono and multilayered two dimensional (2D) nitrogene in which nitrogen atoms are single bonded are studied for energy applications. The otherwise dynamical and thermal stable structures at room temperature, dissociate into triple bonded N_2 molecules at higher temperatures (Fig. 1). From *ab initio* molecular dynamics simulations, the dissociation temperature is found to be decreasing with increasing number of layers (1500 K for single layer and 500 K for six layers). The energy released is large due to the energy difference between single and triple-bonded nitrogen (~ 0.88–1.8 eV/atom). Therefore, the high energy densities calculated for the multilayered structures (~ 6–12.3 KJ/gm) can secure these materials an important position amongst non-nuclear and inorganic high energy density materials known today with comparatively low dissociation temperatures, with the end product being only nitrogen gas.

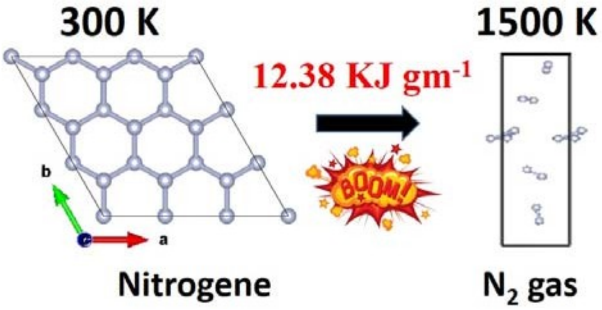

Figure 1: Dissociation of single bonded monolayer nitrogene to molecular N_2, accompanied by a large energy release.

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P41

DFT exploration of magnetic properties in substitutionally doped graphene nanoribbons

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Recent experimental techniques like on-surface synthesis have granted the possibility of obtaining atomically-precise bottom-up graphene nanoribbons (GNRs). In this context, the unprecedented level of control of the overall morphology[1] of the GNRs and of chemical substitution[2] has given rise to the exploration of novel features in these systems such as magnetic properties and topological phases.

Motivated by this, in this work Density Functional Theory simulations are performed to achieve atomic-level insights into the electronic states and the local magnetization of different systems. A set of width-modulated pristine and boron doped GNRs are taken into account. By considering different nanoribbons, the consequences of altering the dopant concentration, dopant location and ribbon morphology are studied. Our results might prove relevant for the design of new experiments to further characterize these materials, as well as for the development of new devices in a wide variety of applications in nanoelectronics and spintronics.

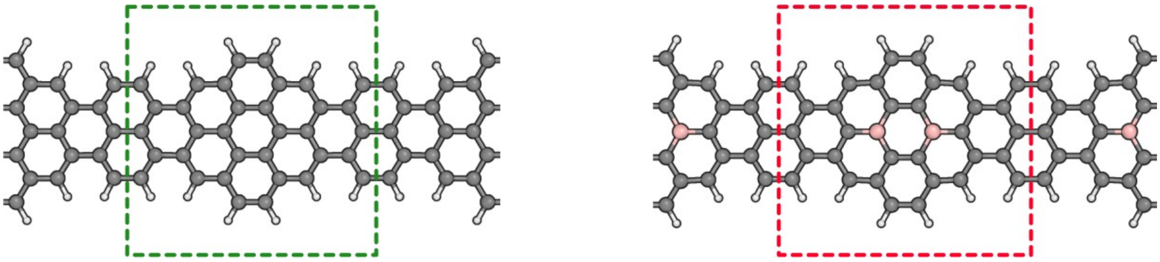

Figure 1: Schematic representation of two of the studied systems and their unit cells. Left: pristine GNR. Right: substitutionally doped GNR.

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P42

Ab initio study of possible metastable occupation of tetrahedral sites in Palladium Hydride compounds

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Palladium hydrides are one of the rare examples of superconducting hydrides at ambient pressure. Even if their critical temperature is around 10 K, they are fascinating superconductors because of their inverse isotope effect: the palladium compound has a larger critical temperature than the hydrogen compound, in clear contradiction with standard electron-phonon superconductors. As shown by Errea et al. [1], this anomalous behavior is induced by the large anharmonicity of the hydrogen vibrations in the octahedral sites they occupy.

In recent times, in a controversial paper [2], high temperature superconductivity was observed in PdH compounds. The authors of the paper measure traces of superconductivity as high as at 54K for PdH if this compound is obtained through fast cooling in the synthesis. If the compound is obtained with slow cooling no superconductivity is observed. Their conclusion is that superconductivity depends strongly on the sites occupied by hydrogen atoms.

In this work we present first principles calculations including anharmonic e.ects within the stochastic self-consistent harmonic approximation (SSCHA) [3] in order to unveil the possible existence of dynamically stable structures with full or partial occupation of tetrahedral sites, which may be metastable. We discuss the implications of these possible structures in superconductivity.

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P43

Molecule contamination effects on nanofriction in layered materials: An ab initio study

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Layered Transition Metal Dichalcogenides (TMDs) have emerged as promising materials for many applications in electronics, optolectronics and photonics, such as photovoltaic devices, lithium batteries, hydrogen evolution catalysis, transistors, photodetectors, DNA detection, memory devices and tribological applications. TMD frictional properties at the atomic scale are particularly relevant in nanoengineerd materials which are at the basis of the aforementioned applications. In this perspective, we conduct a quantum mechanics ab-initio investigation with advanced methods of electronic and phonon analysis on prototypical layered MX2 (M = transition metal and X = chalcogen atom) TMDs with hexagonal structure in the presence of small molecules of contaminants from the atmosphere between two adjacent MX2 layers. We study how the vibrational frequencies of the pristine material are affected by the presence of contaminants, and relate such changes to the nanoscale friction between adjacent layers. We finally obtain guidelines on how to engineer intrinsic friction in TMDs at the nanoscale.

P44

A Functional for Strong Correlation in 1D & 2D

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DFT in its conventional local or semilocal approximations fails dramatically to describe strongly correlated electrons [1]. Restricting to one-particle theories, Natural Orbital Functional (NOF) Theory [2,3] (or 1DMFT) is capable to give an accurate description of such systems [2]. We show the ability of the PNOF7 approximation [2,3] to describe strong correlation in 1D and 2D systems. PNOF7 compares to exact diagonalization, density matrix renormalization group (DMRG), and variational RDM with up to (3,3)-positivity constraints (PQGT') calculations [5] for the 2D Hubbard model (even away from half-filling), which is the prototype to study high-temperature superconductors [4]. In 1D, PNOF7 overcomes OO-AP1roG, recently proposed [6] as an efficient alternative to describe strong correlation in 1D with non-factorial scaling. For the dissociation Hydrogen rings and chains (up to 50 electrons), PNOF7 agrees with DMRG [7], more accurately than coupled-cluster (CC) or moller- plesset (MP2). All calculations were carried out by using DoNOF: Donostia Natural Orbital Functional Software Program [8].

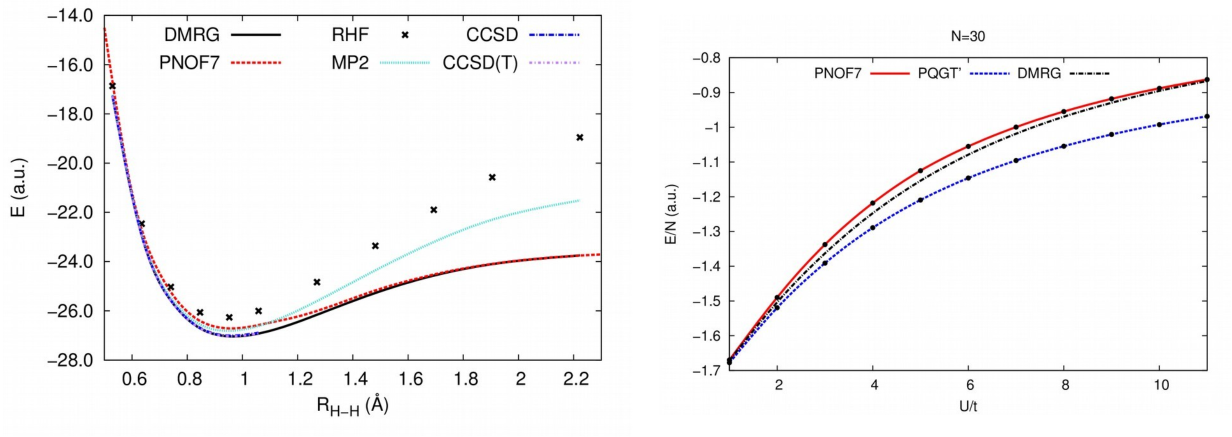

Figure 1: Dissociation of linear H_{50} (left plot), and energies for 6x6 square lattice Hubbard model with 30 electrons for many correlation regimes (right plot).

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P45

PyProcar: A Python library for electronic structure pre/post-processing

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The PyProcar Python package plots the band structure and the Fermi surface as a function of site and/or s,p,d,f - projected wavefunctions obtained for each k-point in the Brillouin zone and band in an electronic structure calculation. This can be performed on top of any electronic structure code, as long as the band and projection information is written in the PROCAR format, as done by the VASP and ABINIT codes. PyProcar can be easily modified to read other formats as well. This package is particularly suitable for understanding atomic effects into the band structure, Fermi surface, spin texture, etc.

PyProcar can be conveniently used in a command line mode, where each one of the parameters define a plot property. In the case of Fermi-surfaces, the package is able to plot the surface with colors depending on other properties such as the electron velocity or spin projection. The mesh used to calculate the property does not need to be the same as the one used to obtain the Fermi surface. A file with a specific property evaluated for each k-point in a k−mesh and for each band can be used to project other properties such as electron-phonon mean path, Fermi velocity, electron effective mass, etc. Another existing feature refers to the band unfolding of supercell calculations into predefined unit cells.

[1] U. Herath *et al.*, arXiv:1906.11387

P46

Excitation Dynamics in Proton-Irradiated Ice

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Ion irradiation of water systems is receiving an increasing attention due to many important applications, such as radiation damage of biological tissues or radiation treatment of tumors, both cases involving systems with a high content of liquid water. For the case of ice, describing its interaction with highly energetic particles at the atomistic and electronic scale is of paramount importance to understand many astrophysical/chemical processes taking place in interstellar dust, comets, asteroids and satellites which are exposed to such particles due to the action of solar wind, cosmic rays or strong magnetospheres.

Here I will show the results of Real-Time Time-Dependent-DFT calculations where the irradiation of ice with highly energetic protons is simulated in real time via Ehrenfest MD, following the excitations of the electronic subsystem in the ice sample promoted by the passing of the proton projectile and describing precisely the change in the trajectory of the proton when hitting the ice target, going beyond the 'constant velocity' approximation that is usually employed when modeling such radiation damage processes. In this way I can not only compute the energy absorbed by the target, but also I can obtain a chemically intuitive picture of which kind of electrons in the system (either 'lone pairs' or 'bonding pairs' electrons) are more likely to get excited, ultimately leading to ionization of the ice target [1].

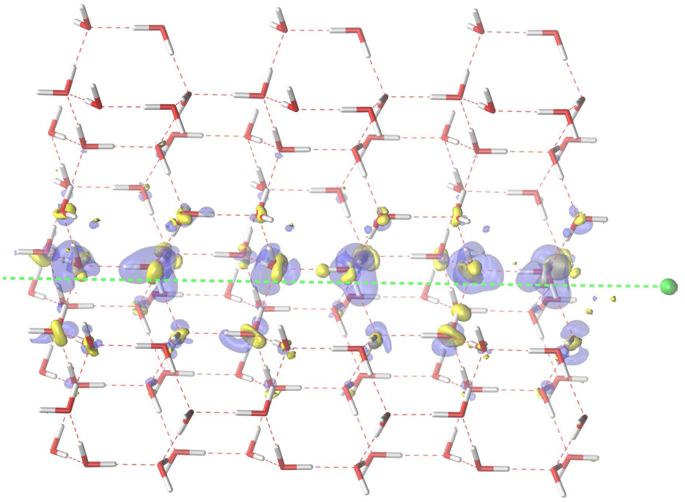

Figure 1: Electron accumulation/depletion (in yellow/blue) caused by the proton irradiation of Ih ice with respect to the ground state.

[1] D. Muñoz-Santiburcio and E. Artacho, *in preparation*.

P47

Tight-Binding Studio: A Technical Software Application to Find the Parameters of Tight- Binding Hamiltonian

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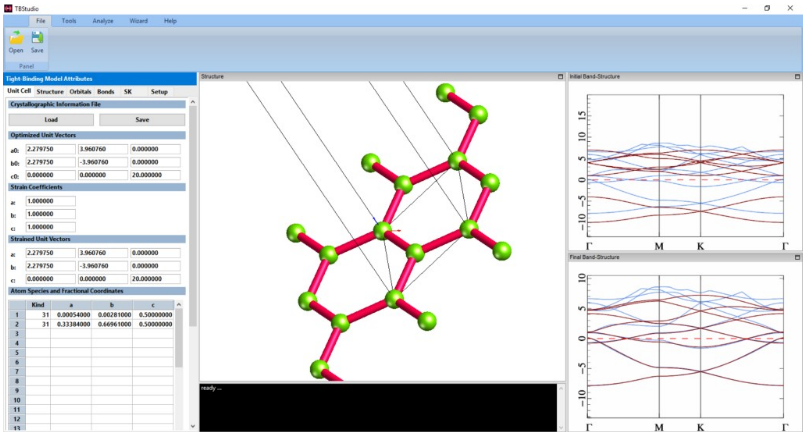
We present Tight-Binding Studio software package for calculating tight-binding Hamiltonian by Slater-Koster method [1] from a set of Bloch energy bands obtained from first principle theories such as density functional theory, Hartree-Fock calculations or Semi-empirical band structure theory. This will be helpful for scientists who are interested in studying electronic properties of structures using Green's function theory in tight-binding approximation. TBStudio is a cross-platform application written in C++ with a graphical user interface design that is user-friendly and easy to work with. This software is powered by Linear Algebra Package C interface library for solving the eigenvalue problems and the standard high performance OpenGL graphic library for real time plotting. TBStudio and its examples together with the tutorials are available for download from tight-binding.com.

The code generator tool inside the TBStudio builds a code for Green's function calculations in other desired programming languages such as C++, C, Fortran, Matlab, Mathematica and Python. Also, one can use the outputs from TBStudio for post- processing in other transport packages such as PyBinding [2], Kite [3], Kwant [4], GPUQT [5], TBTK [6], PythTB [7] and WannierTools [8].



Optimized Unit Vectors
a0: 2.279750 3.960760 0.000000
b0: 2.279750 -3.960760 0.000000
c0: 0.000000 0.000000 20.000000

Strain Coefficients
a: 1.000000
b: 1.000000
c: 1.000000

Strained Unit Vectors
a: 2.279750 3.960760 0.000000
b: 2.279750 -3.960760 0.000000
c: 0.000000 0.000000 20.000000

Atom Species and Fractional Coordinates

	Kind	a	b	c
1	31	0.00054000	0.00281000	0.50000000
2	31	0.33384000	0.66961000	0.50000000
3				
4				
5				
6				
7				
8				
9				
10				
11				
12				

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ready ...
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1: Tight-Binding Studio: a screenshot of an example

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[5] Z. Fan, V. Vierimaa, and A. Harju, Comput. Phys. Commun. **230**, 113 (2018).
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P48

An *ab initio* investigation of a 2D magnet in the presence of graphene

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Discovery of graphene in 2004 marked birth of a completely new area of research – the study of the two-dimensional (2D) materials. Since then, thousands of 2D materials exhibiting a plethora of different properties have been rapidly identified. This fresh and extraordinary field of research is further enlarged by endless ways of vertically stacking different 2D materials, leading to creation of so-called *van der Waals (*vdW) heterostructures. Such structures might improve properties of their constituent layers, and even display new physical phenomena [1].

When discussing vdW heterostructures, of particular interest are crystals containing a 2D magnetic layer. Despite huge experimental efforts, the first 2D magnetic materials have not been obtained until 2017 [2]. The area of 2D magnetic heterostructures is yet unexplored, and offers a lot of new opportunities for discoveries and applications [3]. Here we will focus on the metal phosphorus trisulfides (MPX_3) family of 2D magnets, such as $NiPS_3$.

In this communication we present our software library developed to find supercells of vdW heterostructures, allowing minimisation of the error stemming from the unit-cell-based approach, and thus opening the way for more accurate theoretical investigation of the vdw heterostructures.

We use density functional theory (DFT+U with inclusion of vdW forces) to study the properties of antiferromagnetic $NiPS_3$ and graphene embedded in a heterostructure, taking into account several different mutual orientations of the layers. We discuss and compare magnetic properties of the heterostructure with pristine $NiPS_3$ monolayer, showing that presence of graphene might change the spin arrangements of particular atoms in $NiPS_3$. In addition, the electronic properties of pristine $NiPS_3$ and $NiPS_3$/graphene heterostructure will be presented and compared.

The work is funded by the National Science Center grant no. UMO-2016/23/D/ST3/03446.

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P49

Controlling the properties of the correlated materials

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Correct treatment of the strong correlations inherent to d- and f-shells is of vital importance in many fields of condensed matter physics such as high-Tc superconductors, f-elements, Kondo-systems and others. We combine dynamical mean-field theory (DMFT) and quasiparticle self-consistent GW (QSGW) [1,2] and show on the examples of cuprate superconductors[3], lanthanides[4] and Kondo lattices[5] how the properties of the correlated matter can be controlled via tuning the external conditions.

Understanding why Tc in cuprates is so high has been the subject of numerous investigations and extensive controversy. We explore how displacement of the apical oxygen in La2CuO4 affects the optical gap, spin and charge susceptibilities, and superconducting order parameter. We show that La2CuO4 is a Mott insulator, but small displacements of the apical oxygen drive the compound to a metallic state through a localization-delocalization transition, with a concomitant maximum in d-wave order parameter at the transition. We address the question of whether Nd2CuO4 can be seen as the limit of La2CuO4 with large apical displacements, and we elucidate the deep physical reasons why the behavior of Nd2CuO4 is so different from the hole-doped materials. We shed new light on the recent correlation observed between Tc and the charge transfer gap, while also providing a guide towards the design of optimized high-Tc superconductors.

In Tb, Gd, Dy, we show that the long-accepted monoclinic structure of the "collapsed" high-pressure phases have a 16-atom orthorhombic structure (oF16) not previously seen in the elements, whereas in Nd we show that it has an eight-atom orthorhombic structure (oF8) previously reported in several actinide elements. oF16 and oF8 are members of a new family of layered elemental structures, the discovery of which reveals that the high-pressure structural systematics of the lanthanides, actinides, and group-III elements are much more related than previously imagined. Our results find their confirmation in the experiments using synchrotron x-ray diffraction. We also discuss the magnetic properties of lanthanides at extreme pressure.

In condensed matter, a tremendous effort has been generated to realize the systems with simultaneous charge/spin degrees of freedom that can manifest both Kondo spin quenching and Mott–Hubbard charge localization. Recent developments in controlling densities/temperatures of strongly correlated impurities on surfaces has opened up new possibilities. In this work, we investigate the phase diagram of superlattice structures of f-elements on substrates, assessing required conditions for obtaining Kondo superlattices. We unveil pathways between Kondo quenching and Mott localization, and identify non-trivial charge density waves emerging from the competition of charge localization and Kondo physics.

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P50

Predictive calculations of phonon-limited carrier mobilities in semiconductors

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The ability to predictively compute electron-phonon coupling properties for periodic solids was only recently developed [1].

In this poster, I will present the Boltzmann transport equation within the general framework of the quantum theory of mobility [2].
I will discuss the accuracy limit of ab initio electron-phonon limited calculations of carrier mobilities and show that predictive calculations of electron and hole mobilities require an extremely fine sampling of inelastic scattering processes in momentum space [3].

Such fine sampling calculation is made possible at an affordable computational cost through the use of efficient Fourier-Wannier interpolation of the electron-phonon matrix elements as implemented in the EPW code [4].

Using that interpolation technique, I will present recent findings on the intrinsic electron and hole mobility of silicon [3], wurtzite GaN [5,6], and halide perovskites [7,8].

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P51

A General Approach Towards Continuous Translational Symmetry in Finite Difference Real-Space Calculations

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We have developed a new scheme called the shift operator method to install pseudopotentials on a finite real-space grid that significantly reduces unphysical fluctuations of quantities for fractional grid- point shifts in real space. Instead of interpolating the potential on the grid, this scheme chooses a reference position and use a translation method to represent positions of atoms in real space. This translation is exact for integer grid-point shifts and is designed to minimize the "egg box" effect for fractional grid-point shifts. It provides nonlocal but banded representations for local potentials and is compatible with nonlocal pseudopotential operators. As a demonstration, this scheme is tested in one dimension for three types of potentials: a local ionic potential, a local ionic potential plus a nonlocal operator, and a local ionic potential plus the Hartree and exchange-correlation potential. Fluctuations of examined quantities are reduced by four orders, four orders, and three orders, respectively. This scheme does not require the manipulation of grids and can be easily extended to the three-dimensional case.

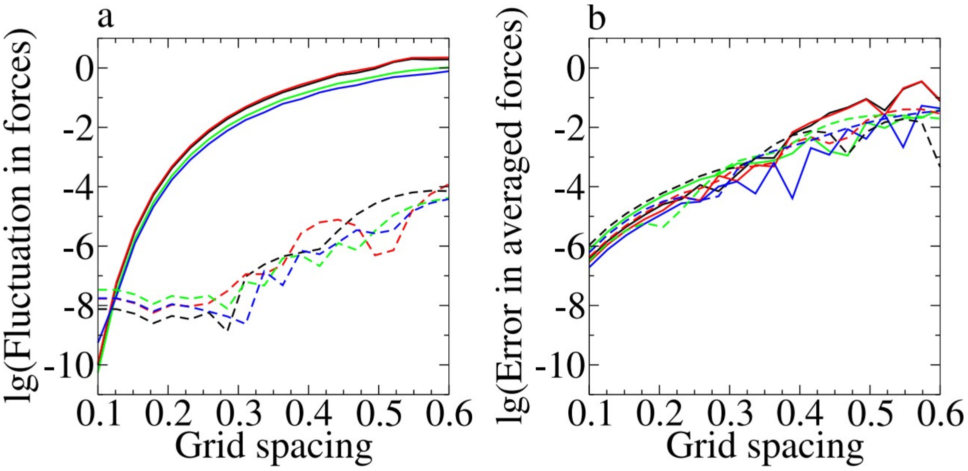

Figure 1 Fluctuations and errors in forces verse the grid spacing for the diatomic system. The absolute error is the average of errors over all fractional shifts. The seven-point stencil is used for the first and second order derivative operators. Color: black, first eigenstate; red, second eigenstate; green, third eigenstate; blue, fourth eigenstate. Line type: solid line, direct interpolation of potential; dashed line, shift operator method. Fluctuations of forces calculated from the shift operator method are reduced by four orders.

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Local mixing in modified Becke-Johnson potential for low-dimensional systems

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The modified Becke-Johnson (MBJ) exchange-correlation potential [1] is known as one of the best for calculations of band gaps of solids using density-functional theory. It is designed as a sum of two terms with a mixing factor *c* which is calculated self- consistently from electronic density and its gradient in the whole unit cell.

In this work we followed the approach of local hybrid functionals [2,3] and evaluated the local mixing *c(r)*. We implemented our method in the Vienna ab-initio simulation package code [4]. We first confirmed that the MBJ band gap values of bulk materials are recovered when using an appropriate averaging of *c(r)* and then calculated electronic properties of semiconductor heterostructures. We obtained correct band gaps in bulk regions also for the heterostructures, in contrast to the PBE [5] functional or the original MBJ potential. The calculated band-oBset values are better than the PBE results and some are comparable with GW values. Finally, we applied a second modification to the MBJ potential which enables us to use it for systems with vacuum, such as slabs or molecules, in contrast to the original version. This makes the MBJ potential applicable to a broader variety of materials, where it might be used to calculate band or HOMO-LUMO gaps with the low computational cost of metaGGA potentials, but possibly still with the accuracy of the original MBJ potential. If the latter goal is met is still a subject of ongoing investigations, but first results promise a clear improvement over the PBE functional.

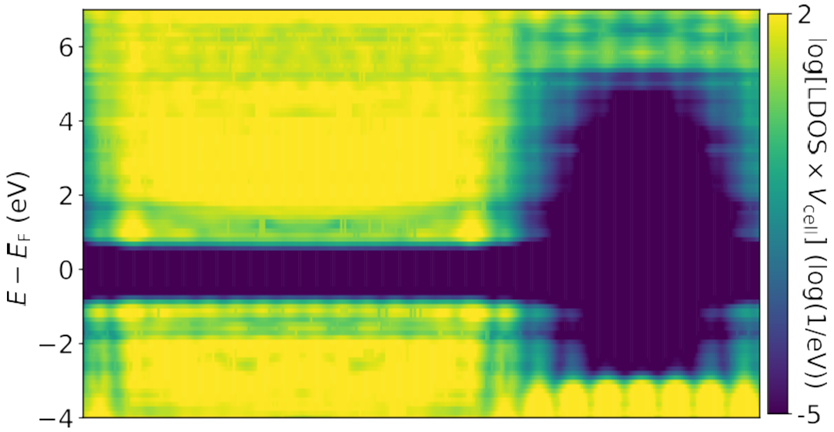

Figure 1: Local density of states of a Si/SiO$_2$ heterostructure calculated with the local MBJ potential.

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P53

Straining the 3fold: Hall viscosity of a New Fermion

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Topological materials are in the spotlight of the Condensed Matter community. One of the most important results on the field has been the development of Topological Quantum Chemistry [1], the formalism that mixes group theory with electronic bands to predict the topological behaviour of materials from symmetry arguments. In this context, several new fermionic excitations, with no analogue on High Energy Physics, were found [2]. These are the so called New Fermions. In this work, we analyse the effect strain has on one of these New Fermions, the 3fold, found on chiral, non-symmorphic Space Group (SG) $P2_13$ as well as in SG $I2_13$.

When considering systems with broken Time Reversal symmetry, one can study hydrodynamic analogues for viscous electron flow [3]. In particular, we compute the non- dissipative viscosity (Hall viscosity) for this New Fermion using Kubo formalism.

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P54

Density functional embedding theory in Gaussian and Plane Waves Formalism

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We present the periodic implementation of the density functional embedding theory (DFET) [1] within the Gaussian and plane waves formalism (GPW) [2]. Based on the unique embedding potential formalism, DFET allows for accurate calculations on the subsystems embedded in the DFT environment, combining accuracy with computational efficiency. DFTET is a top-bottom approach based on the reconstruction of the DFT density of the total system as the sum of the DFT subsystem densities. High-level calculation of the subsystem is more natural and efficient in the local basis, whereas those of the extended systems benefit from the plane waves representation. GPW formalism uses dual basis sets: local Gaussians for orbital expansions and matrix quantities and plane waves for densities and potentials. Thus, it provides a natural framework for the condensed-phase DFET and a seamless connection to molecular quantum chemistry software to be used as high-level solvers.

DFET has been implemented into the CP2K [3] program, which allows for hybrid DFT, RPA and MP2 as high-level methods embedded in GGA DFT. Fig. 1 shows the application of DFET to water adsorption on the 111 surface of magnesium dioxide. Whereas the PBE potential energy curve is way off the full RPA reference, as expected, this at the RPA embedded in PBE almost matches the reference at a dramatically reduced computational price.

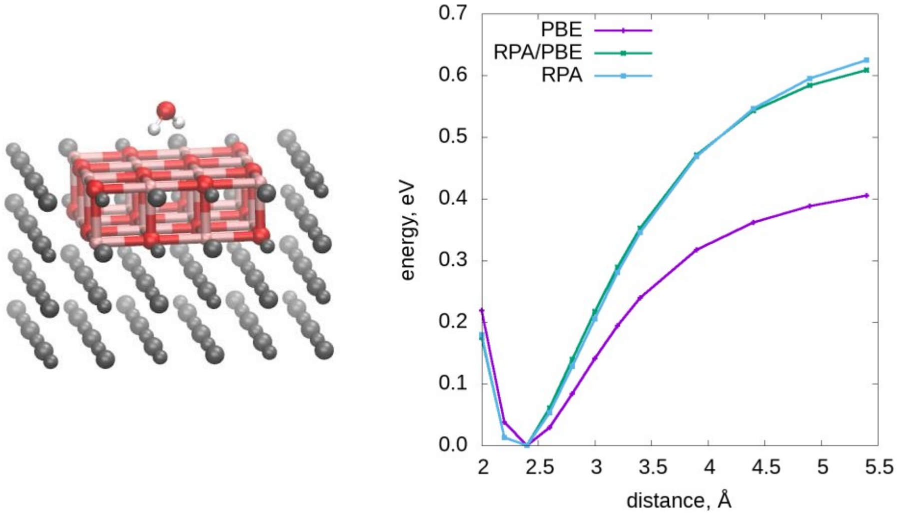

Figure 1: Adsorption of water on 111-surface of magnesium oxide from DFET. Left: system partitioning: gray – environment, red – embedded cluster. Right: potential energy curves: lila – PBE; sky-blue – RPA, green – RPA embedded in PBE.

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P55

N-terminal Graphene-based Nanostructures for Electron Quantum Optical setups

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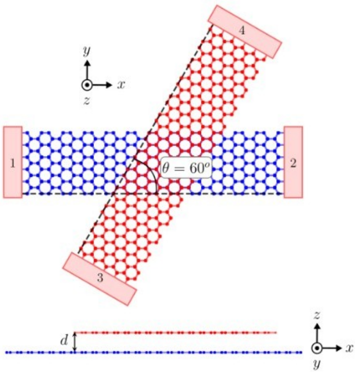
Graphene exhibits many exceptional mechanical and electronic properties that make it attractive for the fabrication of electronic devices at the nanoscale [1], but its gapless spectrum is a major obstacle for carbon-based electronic applications, since the absence of an electronic gap makes it a poor candidate to build logic electronic devices, e.g. field-effect transistor [2]. A gap can be however induced in different ways, among others, via lateral quantum confinement of the electrons, e.g., as it occurs in one-dimensional (1D) graphene nanoribbons (GNRs). On the other hand these GNRs can be produced [3] and manipulated [4, 5] with atomistic precision.

Here we analyze the effect of placing two GNRs one on top of the other interacting via the van-der-Waals interaction (4-terminal device, see Fig.). Previous work based on DFT and Non-equilibrium Green's functions (NEGF) formalism [6] showed that electrons injected from one terminal can be split into two outgoing waves with a tunable ratio that strongly depends on the intersection angle between the ribbons. In this work we complement this by adopting a simple and numerically efficient tight-binding description that captures the essential physics [7]. In addition to the intersection angle, the precise stacking of the device results in a powerful tool to control the direction and intensity of the electron beam. Here we study the electron transport properties in terms of the Scattering matrix, which can be easily computed in the NEGF formalism by means of the generalized Fisher-Lee relations [8], of the different highly-symmetric configurations of crossed GNRs of varying width and edge chiralities, and their possible applications for electron quantum optical setups [9, 10].



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P56

Lattice Dynamics of Cubic $SrTiO_3$: A Simple Way of Temperature-Dependent Phonon Calculations

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Lattice dynamics is one of the most important research subjects in materials science because of its close relation with thermodynamics and transport properties. For some anharmonic crystals where the harmonic approximation fails to describe them well, it is necessary to take into account the lattice anharmonicity. Many studies are devoted to deal with dynamical instabilities while reducing the cost of computing, such as temperature-dependent effective potential (TDEP) method [1] and self-consistent phonon (SCP) theory based method [2]. Cubic perovskite $SrTiO_3$ is one of the well-studied high temperature phase materials, which is dynamically unstable at low temperature. Here, given an example of cubic $SrTiO_3$, we apply the phonon renormalization using only harmonic force constants to obtain the well-defined phonon dispersions at finite temperature. Our final aim is to look for a simple but effective way to automate the temperature-dependent phonon calculations.

All of the density functional theory (DFT) calculations are performed using the VASP code [3]. For phonon calculation, we develop new functions of calculating temperature-dependent phonon properties for Phonopy software [4] and use the interface to ALM software [5] to obtain effective harmonic force constants by fitting approach. The temperature effect to force constants is incorporated by random displacements of atoms from canonical ensemble of harmonic oscillator. By monitoring the harmonic Helmholtz free energy and renormalized phonon frequencies, the computed phonon dispersion free from imaginary frequencies is well converged and obtained. To demonstrate the validity of our approach, we mainly investigate the cubic perovskite structures $SrTiO_3$, which is stable at room temperature. By performing the iterative procedure of our method, we find that all imaginary parts shown at 0K (dashed lines) disappear and the system becomes dynamically stable at 300K (solid lines) as shown in Figure 1, which agrees well with earlier study. In summary, we provide a simpler way to sufficiently describe the phonon dispersion of anharmonic systems at finite temperature by extracting only second-order force constants. We expect that this simple and effective approach can be robust and useful in future with improving algorithms and functions.

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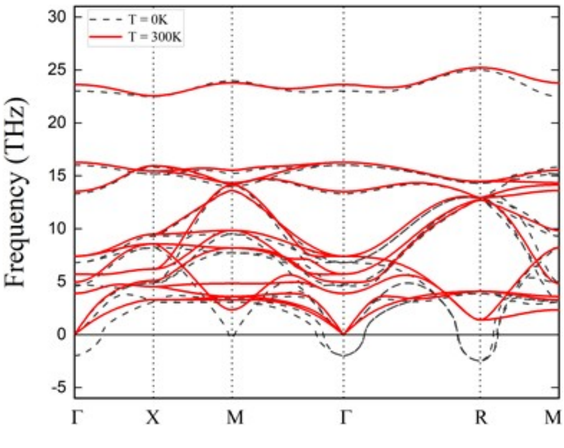

Figure 1: Phonon dispersions at different temperatures

P57

Theoretical study of multivalent ionic transport in spinel host materials

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In the area of sustainable energy storage, multivalent batteries have been attracting considerable attention due to their potential for high energy-density as well as reversibility and abundance benefits. However, a major problem lies in a sluggish kinetics during intercalation at room temperature. This study addresses the ionic conductivity in spinel host materials based on periodic density functional theory (DFT) calculations in order to identify the critical parameters which determine the insertion and extraction of ions. We find that the distribution of cations over octahedral and tetrahedral sites has a decisive influence on the conductivities. Based on our theoretical study, we rationalize the impact of the metal distribution in the host material and the ion concentration on the diffusion process. Furthermore, cathode-related challenges for practical devices will be addressed. Our findings shed light on the fundamental mechanisms underlying ionic conductivity in solid hosts and thus may contribute to improve ion transport in battery electrodes.

The work has been supported by the DFG through Germany’s Excellence Cluster EXC-2154, project 422053626.

P58

Wannier19: an advanced tool for interpolation of Berry curvature and related quantities.

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In this contribution I present my recently-developed code for efficient Wannier interpolation of Berry curvature, orbital magnetic moments and other properties of Bloch bands, as well as the integrated quantities, like anomalous Hall conductivity (AHC), anomalous Nernst effect (ANE), gyrotropic effects and others.

The name “Wannier19” refers to the starting year of the project 2019 and links to the well-known Wannier90 code, which nowadays became a well-established community-driven code[1] for constructing Maximally localized Wannier functions [2]. Wannier90 also includes a post-processing part (postw90.x), where an extensive functionality is implemented, and new effects are constantly being added. However, the methodological aspect still leaves some considerable room for improvement, which is partly hindered by the rigid structure of the Fortran90 code. All this motivated me to start this new python project, and in this poster I will present my advances in this direction.

So far the main advantages of Wannier19 over Wannier90 are:

- employing fast fourier transform (FFT) instead of the “slow” FT
- recursive adaptive refinement algorithm to improve integration of diverging quantities.
- account of symmetries help to reduce integration to the irreducible part of the Brillouin zone
- more efficient algorithms, in particular speeding up in case of for
  - evaluation of AHC for multiple Fermi levels
  - minimal-distance replica selection method
- written in object-oriented Python3, which offers advantages:
  - the new quantities can be implemented in a laconic way
  - the new implemented algorithms affect all quantities.

As a result, right now the code can be used for extremely fast and accurate calculations of AHC and ANE. Among the features planned for implementation in the nearest future (probably implemented by the time of the conference) are low-field anomalous Hall effect in the non-Abelian formulation, to account for systems with PT symmetry which have Kramers degeneracy everywhere in kspace.

Wannier19 is an open-source project [3] and everyone is kindly invited to use it and collaborate on the development.

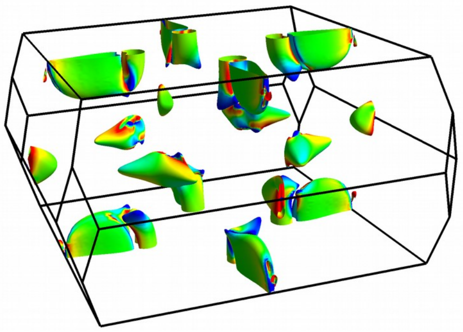

Figure 1: (Color online) Wannier19 also has a routine to produce input for the Fermisurfer tool [M.Kawamura, Comp. Phys. Commun 239, 197 (2019)] to produce plots of the Fermi surface(FS) coloured by any quantity. As an example, the figure shows the FS of a magnetic Weyl semimetal PrAlGe colored by the value of Berry curvature Ω_z divided by Fermi velocity. After performing the FS integral, this gives the magnitude of the ANE.

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P59

Stability of π-electron-deuterium coupled ordering in hydrogen-bonded molecular conductors κ-D3(Cat-EDT-TTF/ST)2

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Charge ordering (CO) is a phenomenon characterized by a collective electron transfer, producing charge disproportionation between inter-molecular sites or ionic sites. If the CO transition occurs associated with the breaking of inversion symmetry, the system may be ferroelectric. A fundamental problem is that the CO phases often seen experimentally and extensively studied theoretically, are not structurally stable within the standard DFT approach, especially in molecular materials. Namely, even when we perform structural optimization starting from the experimentally observed low temperature structure with CO, the optimized structure becomes that of the high-temperature phase where charge disproportionation is absent.

Here we study a class of molecular crystals based on catechol with ethylenedithiote- tetrathiafulvalene, Cat-EDT-TTF, and its selenium-substituted analogue, Cat-EDT-ST [1]. In the electronic and structural properties, hydrogens and π-electrons are strongly linked, through the hydrogen bonding in their constituent molecular unit [2-4]. In the D samples of κ-D3(Cat-EDT- TTF/ST)2 (D-S/D-Se), a first-order phase transition occurs associated with a large structural change at the transition temperature (Tc) of 182 K and 185 K in D-S and D-Se, respectively [1]. The magnetic susceptibility decreases sharply below Tc resulting in a nonmagnetic ground state. In this work, we compare the GGA-PBE functional with a range-separated hybrid functional by Heyd-Scuseria-Ernzerhof (HSE06) [5], and investigate the stability of the CO phases in D-S and D-Se. The latter formalism enables us to improve the exchange-correlation energy by mixing the non-local exact (Fock) exchange and semi-local exchange energy functional used in conventional DFT approaches within GGA. We found that, using the experimental crystal structure, both GGA and HSE06 calculations show CO but with a larger degree of charge disproportion in HSE06 functional closer to the experiments [6]. Moreover, using HSE06, an insulating band structure obtained for D-S. By performing structural optimization with HSE06, the central C=C bond lengths that are sensitive to the degree of charge disproportionation are well reproduced, whereas GGA fails in stabilizing the CO state. We also propose possible patterns of D ordering and show a stable noncentrosymmetric CO phase which has close energy
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P60

Computational insight on the energy transfer properties of small noble metal nanoclusters

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The study of physical and chemical properties of ultra-small (< 2 nm) noble metal nanoclusters has become one of the most exciting and promising fields in nanoscience. The intrinsic quantum confinement effects given by the small dimension, together with the unconventional stable geometries and the possibility to control the stoichiometry with atomic precision, give them unique properties in terms of optical, magnetic and catalytic features.[1]

In this work we investigated the mechanism behind the enhancement of the photoluminescence yield of erbium ions implanted in silica, when small gold or silver nanoclusters are also implanted. Indeed, experimental evidences show that this enhancement is directly related to the presence of small Au or Ag nanostructures, it depends on cluster concentration, nature and size, and, in some specific cases, it can be activated by choosing the correct annealing atmosphere. [2], [3], [4]

Therefore, we employed Density Functional Theory (DFT) and Time Dependent DFT (TDDFT) calculations, to study the energy level distributions of several M20 and M12 (M = Au, Ag or a 1:1 Au/Ag alloy) model nanostructures, finding that both M20 and M12 nanostructures can pump the 4I13/2 erbium emitting level through a triplet state assisted Dexter-like energy transfer, acting as in an antenna- lanthanide complex. This transfer resulted to be more favourable using silver rather than gold and considering M20 geometries rather than the smaller ones. Furthermore, we proved that Au20 and Au12 have weaker absorption intensities and worst energy levels alignment with respect to the silver-based structures and thus, their presence can reduce or even suppress the triplet state assisted energy transfer.

In order to include the effect of a defected solid matrix, we added an extra H3SiO - anion in all tested systems and tried to understand how these defects can be involved in the energy transfer process. We demonstrated that the presence of this anion heavily modifies the excited states energy distribution of Au-based nanoclusters, sometimes bringing the first triplet state levels below the threshold of the erbium emitting level and suppressing the energy transfer, while only weakly affect Ag-based nanostructures. This is way more evident in M12 clusters. Globally, all our results qualitatively agree with the experimental observations [3], [4] and support the hypothesis of an excited states assisted energy transfer to the 4I13/2 erbium emitting level.

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Computing the Self-Consistent Field in Kohn- Sham Density Functional Theory

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A new framework is presented for evaluating the performance of self-consistent field methods in Kohn–Sham density functional theory (DFT) [1]. The aims of this work are two-fold. First, we explore the properties of Kohn–Sham DFT as it pertains to the convergence of self-consistent field iterations. Sources of inefficiencies and instabilities are identified, and methods to mitigate these difficulties are discussed. Second, we introduce a framework to assess the relative utility of algorithms in the present context, comprising a representative benchmark suite of over fifty Kohn–Sham simulation inputs, the scf-x_n suite [2]. This provides a new tool to develop, evaluate and compare new algorithms in a fair, well-defined and transparent manner.

This work is published as a topical review [1]. As such, the article is accessible to a variety of different backgrounds, and constitutes, at least in part, a pedagogical resource. The contained analysis, test suite, and benchmarking pipeline is designed to assist future method development.

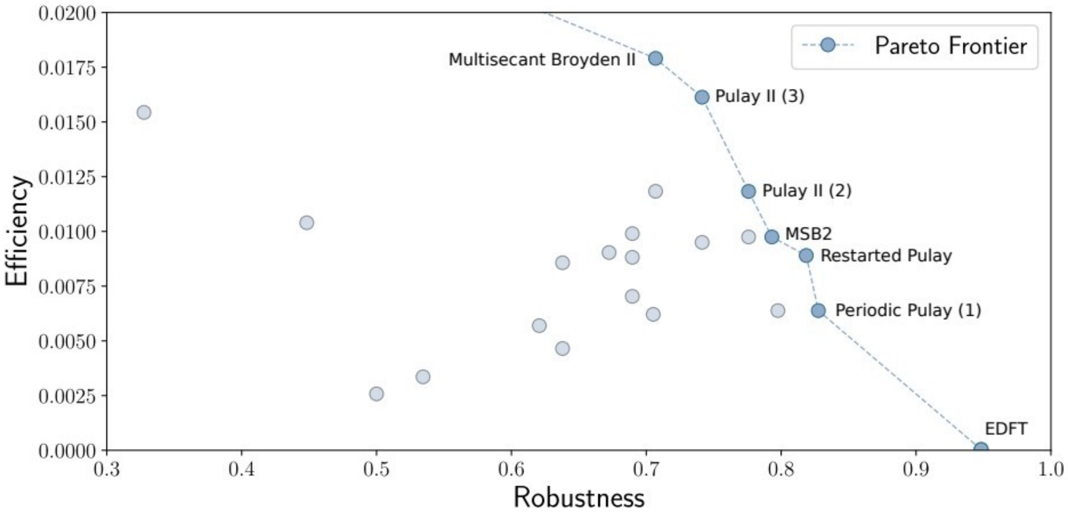

Figure 1: The utility of algorithms (nodes ●) across a test suite [2] as a function of two utility measures: robustness and efficiency. The Pareto frontier defines, in a certain sense, the set of optimal algorithms in the present context.

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[2] N. Woods., DOI: 10.5281/zenodo. 3344540

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Understanding atomic and electronic structure across the family of 2D transition metal dichalcogenides

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Layered transition metal dichalcogenides (TMDs) of chemical composition MX2 (M = transition metal; X = S, Se, or Te) represent a broad family of materials with diverse electronic properties, including metals, insulators, as well as more complex states such as the charge-density-wave (CDW) and superconducting phases. More recently, the possibility of realizing single- and few-layer TMDs has brought the two- dimensional (2D) forms of these materials into the spotlight of prospective application in electronics, optoelectronics and beyond [1]. We review the “periodic table” of TMDs attempting to reveal systematic trends and develop chemical intuition across this family of 2D materials. More specifically, in this presentation we address the following problems. Using a Wannier function approach, we investigate the relevance of the crystal and ligand fields in determining the relative stability of 1T and 1H polymorphs as a function of the filling of the d-shell in 2D TMDs [2]. Then, we present a unified picture of lattice instabilities in metallic TMDs that describes both the CDW phases and the strong-coupling scenario resulting in the formation of metal-metal bonds (as e.g. in the dimerized 1T’ phases) [3].

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Theoretical approach to II-VI nanoclusters in ionic liquids

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Unique and attractive properties have been predicted for II-VI type based semiconductor nanoclusters within the field of nanotechnology. However, the low reaction kinetics within the usual solvents gives only the thermodynamic control during their production process, making the obtention of different metastable polymorphs of such materials extremely difficult [1]. The use of ionic liquids as solvents is expected to overcome this problem, as they have already proved to increase the reaction kinetics in various chemical systems [2]. The complexity and size of the system requires an efficient simulation protocol, which is established in this work. Taking as reference the semiconductor (ZnS)12 nanocluster and the [EMIM][EtSO4] ionic liquid, we evaluate the performance of various force-fields. Then, classical molecular dynamics are carried out, showing the formation of a structured IL solvation shell around the nanocluster with no exchange of molecules for at least 10 ns. The ab inito calculations agree with the previous observations, justifying the reliable use of an implicit solvation model to simulate the molecules of the ionic liquid that do not conform the first solvation shell. We assess the performance of several exchange-correlation functionals, basis-set and hydrogen bond acidities of the implicit solvation model, and identify the most adequate combination based on geometrical and energetic criteria. In summary, we stablish the following theoretical simulation protocol to study the stability and dynamics of II-VI type based semiconductor nanoclusters solvated by ionic liquids efficiently: first, obtain the final configuration of the nanocluster-ionic liquid system via classical molecular dynamics and second, carry out ab initio calculations taking the final configuration of the nanocluster and the first solvation shell from the previous step, and simulate the rest of the ionic liquid by an implicit solvation model.

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