BOOK OF ABSTRACTS

SCIENTIFIC PROGRAM

Lecture Hall John von Neumann, Patrick M.S. Blackett Institute (San Domenico)

Saturday July 6th

19:30-21:30 *Dinner in affiliated restaurant*

21.30 **Meet up at the Marsala Room in I.I. Rabi Institute (San Rocco)**

Sunday July 7th

09:00-12:50 **Morning Session,** Chairs: *Alessandro Molle, Antonio Cricenti*

09:00-09:20 *Antonio Cricenti, Alessandro Molle* **Opening of the school: Welcome to Erice**

09.20-10.00 *Friedhelm Bechstedt* Ab-initio description of optical properties of bulk, layers, surfaces and nanostructures (1)

10.00-10.40 *Athanasios Dimoulas* Epitaxial 2D materials with non-trivial topology (1)

10:40-11:00 *Ygit Sozen* Massive parallel mechanical exfoliation: a scalable and low-cost production method for few-layer 2D materials

11:00-11:20 **Coffee break (Poster Mounting)**

11:20-12:05 *Harold Zandvliet* Germanene: a monoelemental 2D topological insulator

12.05-12.50 *Yves Borensztein* Multi-technique study of some Xenes films: growth, structure, reactivity and optical properties

13:00 ***Lunch (affiliated restaurants)***

16:00 – 19:50 **Evening Session,** Chairs: *Yves Borensztein, Harold Zandvliet*

16:00-16:45 *Christoph Cobet* In-situ polarization optics in electrochemistry

16:45-17:30 *Francesco Bisio* Ellipsometry spectroscopy of low-dimensional materials

17:30 - 17:45 **Coffee break (Poster mounting)**

17:45-18:25 *Friedhelm Bechstedt* Ab-initio description of optical properties of bulk, ayers, surfaces and nanostructures (2)

18:25-19.05 *Athanasios Dimoulas* Epitaxial 2D materials with non-trivial topology (2)

19:05-19:50 *Olivia Pulci* Electronic and optical properties of 2-D materials: effect of gating, twisting, and of the substrate.

20:00 ***Dinner (selected restaurants)***

21.30 ***Meet up at the Marsala Room in I.I. Rabi Institute (San Rocco)***

Monday July 8th

09:00 - 13:00 **Morning Session,** Chairs: *Athanasios Dimoulas, Friedhelm Bechstedt*

09:00-09:40 *Juan Sierra* Spintronics and thermoelectrics based on 2d van der Waals Heterostructures (1)

09.40-10.20 *Doron Naveh* Optoelectronics based on 2D materials (1)

10.20-10.40 *Julian Plaickner* Synchrotron-based VUV ellipsometry on passivated Si samples and Al_2O_3 for optical thin film metrology

10:40-11:00 *Esteban Zamora* Roll-to-Roll Exfoliation for Anisotropic Films of 2D Materials

11:00 - 11:30 **Coffee break & Poster session**

11:30-12:15 *Francesco Buatier de Mongeot* Nanopatterning 2D semiconducting layers for large-scale photon harvesting and nanoelectronics

12:15-13:00 *Kenan Gundogdu* Room Temperature Superfluorescence in Perovskites and Its Implications for Quantum Materials

13:00 ***Lunch (affiliated restaurants)***

16:00 - 19:50 **Evening Session,** Chairs: *Francesco Buatier de Mongeot, Kenan Gundogdu*

16:00-16:45 *Luis Mochan* Homogenization of multicomponent metamaterials

16:45-17:30 *Kjeld Pedersen* Optical properties of metallic nanowires.

17:30-18:00 **Coffee break and Poster Session**
18:00-18:40 *Juan Sierra* Spintronics and thermoelectrics based on 2d van der Waals Heterostructures (2)
18.40-19.20 *Doron Naveh* Optoelectronics based on 2D materials (2)
19.20-19.50 *Antonio Cricenti* Optical nanospectroscopy for bioanalysis
20:00 ***Dinner***
21.30 ***Meet up at the Marsala Room in I.I. Rabi Institute (San Rocco)***

Tuesday July 9th

09:00 - 12:45 **Morning Session,** Chairs: *Doron Naveh, Luis Mochan, Kjeld Pedersen*
09.00-09.40 *Cinzia Casiraghi* Overview on 2D Material-based Inks: from Fundamentals of Colloidal Chemistry to Applications (1)
09:40-10:20 *Sang-Hoon Bae* Fabrication of van der Walls stacks (1)
10:20-10:40 *Simone Grillo* Tunable Second Harmonic Generation in 2D Materials from First-Principles
10:40-11:00 *Renebeth Payod* Analysis of the Absorption Resonances between Carbynes and Cyclo[n]carbons: a tight-binding approach
11:00-11:30 **Coffee break & Poster Session**
11:30-12:15 *Luca Vattuone* Experimental observations of the acoustic surface plasmon: from Electron Energy Loss Spectroscopy to Hyperthermal atom scattering
12:15-13:00 *Christoph Tegenkamp* Proximity coupling effects in epitaxial 2D graphene-based systems
13:00 ***Lunch (affiliated restaurants)***
16:00 - 19:40 **Evening Session,** Chairs: *Christoph Tegenkamp, Juan Sierra*
16:00-16:45 *Vyacheslav Silkin* Low-energy collective electronic excitations at metal surfaces and layered materials
16:45-17:30 *Carmen Munuera* Strain engineering of 2d materials
17:30-18:00 **Coffee break & Poster Session**
18:00-18:40 *Cinzia Casiraghi* Overview on 2D Material-based Inks: from Fundamentals of Colloidal Chemistry to Applications (2)
18.40-19.20 *Sang-Hoon Bae* Fabrication of van der Walls stacks (2)
19:20-19:40 *Domenico Corona* Self-consistent Hubbard parameters in doped layered transition-metal oxides for sodium-ion batteries
20:00 ***Dinner***
21.30 ***Meet up at the Marsala Room in I.I. Rabi Institute (San Rocco)***

Wednesday July 10th

09:00 – 13:00 **Morning Session,** Chairs: *Dietrich Zahn, Carmen Munuera*
09.00-09.45 *Junji Yuhara* Growth of group 14 elemental post-graphene materials
09:45-10:30 *Jonhathan Bradford* Molecular Beam Epitaxy of 2D Materials for Deep-UV Optoelectronics
10:30-11:00 **Coffee break & Poster Session**
11:30-12:15 *Zdenek Sofer* 2d silicon, germanium, and pnictognes by chemical methods
12:15-13:00 *Alessio Lamperti.* Strategies for tuning the CVD synthesis of 2D transition metal dichalcogenides in a hot-wall tube reactor
13:00 ***Lunch (affiliated restaurants)***
15:00 ***Excursion to Segesta or Selinunte or Mothia, take with you solar cream, cap, water, snacks***
20:00 ***Social Dinner***

Thursday July 11th

09:00 – 13:00 **Morning Session, Chairs:** *Cinzia Casiraghi, Norbert Esser*
09:00-09:45 *Mark Hersam* Mixed-Dimensional Heterostructures for Electronic and Energy Technologies
09:45-10:30 *Aldo Di Carlo* MXenes and other two-dimensional materials in new generation photovoltaics
10:30-11:00 **Coffee break & Poster Session**
11:00-11.45 *Christoph Gadermeier* Ultra-fast spectroscopy of 2d materials
11:45-12:30 *Norman Tolk* Point defect and proximal interface induced modification of Er^{3+} optical transitions in single crystal Er_2O_3
13:00 ***Lunch (affiliated restaurants)***
16:00 - 19:45 **Evening Session,** Chairs: *Christoph Gadermeier, Olivia Pulci*

16:00-16:45 *Norbert Esser* Raman Spectroscopy at Surfaces and 2D Metallic Layers
16:45-17:30 *Dietrich Zahn* Plasmon-enhanced Raman Spectroscopy of Low-dimensional Semiconductors
17:30-17:50 **Coffee break**
17:50-18:35 *James Ingham* The application of artificial intelligence and machine learning to the analysis of spectral images
18.35-19.05 *Alessandro Molle* Xenes: from growth to applications
19:05-19:45 *Antonio Cricenti, Alessandro Molle* **Young Researcher Award and Closing Remarks**
20:00 ***Dinner***
21.30 ***Meet up at the Marsala Room in I.I. Rabi Institute (San Rocco)***

Friday July 12th : Departure (check your schedule time at San Rocco hall)

INVITED TALKS

Tutorials

Athanasios Dimoulas, NCSR-D, Democritos, Athens, Greece *Epitaxial 2D materials with non-trivial topology*
Sang-Hoon Bae, Washington University in St. Louis, USA *Fabrication of van der Walls stacks*
Cinzia Casiraghi, University of Manchester, UK *Overview on 2D Material-based Inks: from Fundamentals of Colloidal Chemistry to Applications*
Friedhelm Bechstedt, University of Jena, Germany *Ab-initio description of optical properties of bulk, layers, surfaces and nanostructures*
Doron Naveh, Bar Ilan University, Tel Aviv, Israel *Optoelectronics basedon 2D materials*
Juan Sierra, ICN2, Barcelona, Spain *Spintronics and thermoelectrics based on 2d van der waals heterostructures*

Linear, non-linear, and ultra-fast optics

Norbert Esser, ISAS, Berlin, Germany *Raman Spectroscopy at Surfaces and 2D Metallic Layers*
Antonio Cricenti, CNR-ISM, Italy *Optical nanospectroscopy for bioanalysis*
Yves Borensztein, CNRS - Sorbonne Universite Paris – France *Multi-technique study of some Xenes films: growth, structure, reactivity and optical properties*
Francesco Buatier de Mongeot, University of Genoa, Italy *Nanopatterning 2D semiconducting layers for large-scale photon harvesting and nanoelectronics*
Dietrich Zahn, Chemniz Univeristy, Germany *Plasmon-enhanced Raman Spectroscopy of Low-dimensional Semiconductors*
Kjeld Pedersen, Aalborg University, Denmark *Optical properties of metallic nanowires.*
Christoph Cobet, Linz School of Education, Austria *In-situ polarization optics in electrochemistry*
Kenan Gundogdu, NCSU Physics, Raleigh, USA *Room Temperature Superfluorescence in Perovskites and Its Implications for Quantum Materials*
Christoph Gadermeier Politecnico Milano, Italy *Ultra-fast spectroscopy of 2d materials*
Norman Tolk, Vanderbilt University, USA *Ultrafast and nonlinear optical spectroscopy*

Emerging 2D Materials and nanomaterials

Harold Zandvliet, University of Twente, Netherlands Germanene: a monoelemental 2D topological insulator
Junji Yuhara, University of Nagoya, Japan *Growth of group 14 elemental post-graphene materials*
Alessio Lamperti, CNR-IMM, Italy *Strategies for tuning the CVD synthesis of 2D transition metal dichalcogenides in a hot-wall tube reactor*
Jonathan Bradford, University of Nottingham, UK *Molecular Beam Epitaxy of 2D Materials for Deep-UV Optoelectronics*
Olivia Pulci, University of Rome Tor Vergata, Italy *Electronic and optical properties of 2-D materials: effect of gating, twisting, and of the substrate*
Zdenek Sofer, University of Chemistry and Technology of Prague, Czech Republic *2d silicon, germanium, and pnictognes by chemical methods*
Luis Mochan, UNAM, Mexico *Homogenization of multicomponent metamaterials*

Applications

Carmen Munuera, CSIC, Madrid, Spain *Strain engineering of 2d materials*
James Ingham, University of Liverpool, UK *The application of artificial intelligence and machine learning to the analysis of spectral images*
Aldo Di Carlo, CNR-ISM, Italy *MXenes and other two-dimensional materials in new generation photovoltaics*
Mark Hersam, Northwestern University, IL, USA *Mixed-Dimensional Heterostructures for Electronic and Energy Technologies*
Alessandro Molle, CNR-IMM, Italy *Xenes: from growth to applications*

Plasmonics

Luca Vattuone, University of Genoa, Italy *Experimental observations of the acoustic surface plasmon: from Electron Energy Loss Spectroscopy to Hyperthermal atom scattering*
Vyacheslav M. Silkin, UPV-EUH, Spain *Low-energy collective electronic excitations at metal surfaces and layered materials*
Christoph Tegenkamp, TU Chemnitz, Germany *Proximity coupling effects in epitaxial 2D graphene-based systems*
Francesco Bisio, CNR-SPIN, Italy Ellipsometry spectroscopy of low-dimesniosnal materials

ORDINARY TALKS

Ygit Sozen, CSIC, Spain *Massive parallel mechanical exfoliation: a scalable and low-cost production method for few-layer 2D materials*
Renebeth Payod, University of Twente, Netherlands *Analysis of the Absorption Resonances between Carbynes and Cyclo[n]carbons: a tight-binding approach*
Simone Grillo, University of Rome Tor Vergata, Italy *Tunable Second Harmonic Generation in 2D Materials from First-Principles*
Domenico Corona, University of RomeTor Vergata, Italy *Self-consistent Hubbard parameters in doped layered transition-metal oxides for sodium-ion batteries*
Esteban Zamora, CSISC, Spain *Roll-to-Roll Exfoliation for Anisotropic Films of 2D Materials*
Julian Plaickner, Technische Universität Berlin, Germany *Synchrotron-based VUV ellipsometry on passivated Si samples and Al_2O_3 for optical thin film metrology*

POSTERS

Matteo Gardella, CNR-IMM, Italy Synthesis of large-area MoS2 films via CVD and L-CVD
Matteo Gradanti, University of Milano Biocca, Italy 1) Chiral photocurrents and photogalvanic effect in bidimensional materials for photonics devices based on topological materials; 2) Study of the optical properties of epitaxial heterostructures based on V-group semiconductors for photovoltaic applications
Simone Brozzesi, University of Rome Tor Vergata, Italy Moiré-induced Dirac cones replicas and minigaps opening in graphene/hBN superlattices
Alessia Muroni, University of Rome Tor Vergata, Italy Unveiling the optical secrets of ice sufaces: insights from advanced computational approaches
Vasil Saroka, University of Rome Tor Vergata, Italy Hydrogenated graphene superlattices: electronic and optical properties
Esra van't Westende, University of Twente, Netherlands Interaction of topological edge states in germanene nanoribbons
Aviv Schwarz, Bar Ilan Univ, Tel Aviv, Israel Thiol-Based Defect Healing of WSe_2 and WS_2
Rajesh Chennuboina, University of Genoa, Italy Maskless synthesis of van der Waals heterostructure and plasmonic arrays engineered for light harvesting on large area templates

ORAL SESSIONS

Ab-initio description of optical properties of bulk, layers, surfaces and nanostructures

Friedhelm Bechstedt
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In the last decades, based on first principles, theoretical and computational schemes have been developed to allow not only for the description and understanding but also the prediction of optical properties of matter, e.g. novel materials as well as novel atomic geometries such as nanostructures in zero, one or two dimensions. The progress made also by the EPIOPTICS community and the basic methods applied will be reported in this talk.
In general, a three-step procedure (see Fig. 1) is applied to describe optical spectra via the dielectric function in a wide frequency range and for given light polarization [1]. (i) As an important ingredient of a parameter-free treatment the atomic geometry of the investigated bulk crystal, two-dimensional material layer/surface/interface, one-dimensional wire arrangement or zero-dimensional nanocrystal is calculated by minimizing the total energy within the density functional theory with a certain exchange-correlation functional. (ii) To overcome the gap underestimates of the accompanying Kohn-Sham electronic structure, in a second step, the formation of quasiparticles in the interacting electronic system after photonic excitation is considered. (iii) In the third step the mainly screened attraction of the excited quasielectrons and quasiholes, the real or virtual formation of excitons, is taken into account. Several examples for application of the combined approaches are presented to illustrate the predictive power and accuracy of the methods. Among them are several optical spectra, e.g. absorption spectra as displayed in Fig. 1.

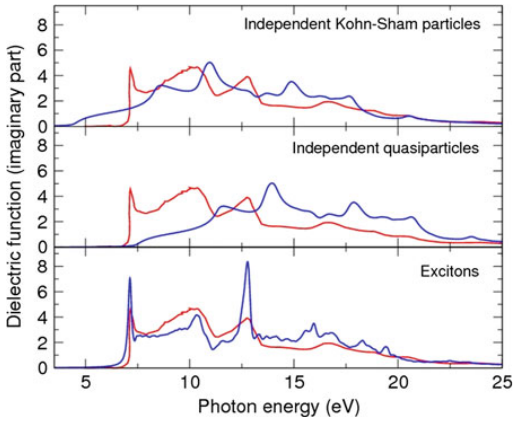

Figure 1. Dielectric function of rs-MgO (blue line) calculated in three different approximations on many-body effects [2] and compared with a measured spectrum (red line) [3].

References:

[1] F. Bechstedt, Many-Body Approach to Electronic Excitations (Springer, Berlin, 2015)
[2] A. Schleife et al., Phys. Rev. B **80**, 035112 (2009)
[3] M.L. Bortz et al., Phys. Scr. **41**, 537 (1990)

Epitaxial 2D materials with non-trivial topology

A Dimoulas

Institute of Nanoscience and Nanotechnology, NCSR DEMOKRITOS, 15341, Athens, Greece

Abstract

In this tutorial, first a general review of molecular beam epitaxy (MBE) basics with a particular focus on 2D materials and van der Waals heterostructures will be presented. Emphasis will be given on the merits of MBE compared to other thin film deposition techniques. Subsequently, the focus will be on the influence of the substrate and in-situ surface preparation techniques on the structural quality and physical properties of the 2D materials. In-situ surface analytical techniques will be discussed such as STM and RHEED for the imaging of surfaces with atomic resolution and ARPES for the imaging of the electronic band structure. Particular attention will be given to 2D materials with non-trivial topology in reciprocal space such as topological insulators [1], T_d-$MoTe_2$ Weyl semimetals [2] (Fig.1) and $HfTe_2$, $ZrTe_2$ Dirac semimetals [3] (Fig. 2). Similarly, ferromagnetic 2D metals (e.g $Cr_{1+\delta}Te_2$, Fe_xGeTe_2) [4, 5] with skyrmion topological structures in real space will be discussed. Combinations of topological materials with 2D metallic ferromagnets can enhance the charge-to-spin conversion resulting in all-electrical control of magnetization switching (Fig. 3) for energy-efficient magnetic memory devices.

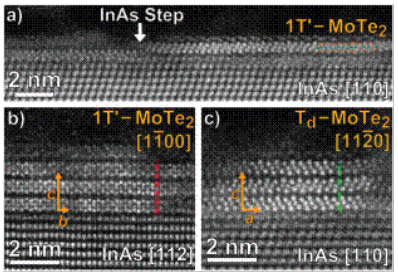

Fig.1 After Ref [2] MBE growth of Weyl semimetal orthorhombic non-centrosymmetric phase T_d-$MoTe_2$.

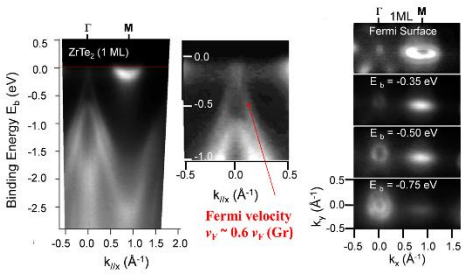

Fig. 2 After Ref [3] In-situ ARPES of MBE grown 1T-$ZrTe_2$ showing massless Dirac fermions at the zone center

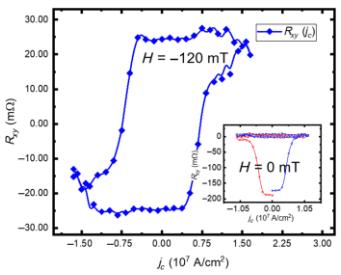

Fig.3 After Ref [4] all-electrical partial magnetization reversal in Bi_2Te_3/$Cr_{1+\delta}Te_2$ heterostructures

References:

[1] S. Fragkos et al., *Phys. Rev. Mater*. (2021) **5**, 014203

[2] P. Tsipas et al., *Adv. Funct. Mater. (*2018), 1802084.

[3] P. Tsipas et al., *ACS Nano* **12** (2018) 1696

[4] N. Figueiredo-Prestes et al., Physical Review Applied (2023) 19, 014012

[5] E. Georgopoulou-Kotsaki et al., *Nanoscale* (2023) **15**, 2223

Massive parallel mechanical exfoliation: a scalable and low-cost production method for few-layer 2D materials

Yigit Sozen[1,*], Juan J. Riquelme [1], Yong Xie[2], Carmen Munuera[1], Andres Castellanos-Gomez[1]

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Scientific Session: Nanofabrication & Nanomanupilation
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We present a method for scaling up the production of few-layer flakes of 2D materials via mechanical exfoliation. Using a roll-to-roll setup and an automatized, massive parallel exfoliation process, adhesive tapes with a high density of few-layer van der Waals materials are produced. The technique allows for obtaining a good trade-off between large lateral size and excellent area scalability, while also maintaining low cost. The potential of the method is demonstrated through the successful fabrication of field effect transistors and flexible photodetectors in large batches. This low cost method to produce large area films out of mechanically exfoliated flakes is very general and it can be applied to a variety of substrates and van der Waals materials and, moreover, it can be used to combine different van der Waals materials on top of each other. Therefore, we believe that this production method opens an interesting avenue for fabrication of low-cost devices while maintaining a good scalability and performance.

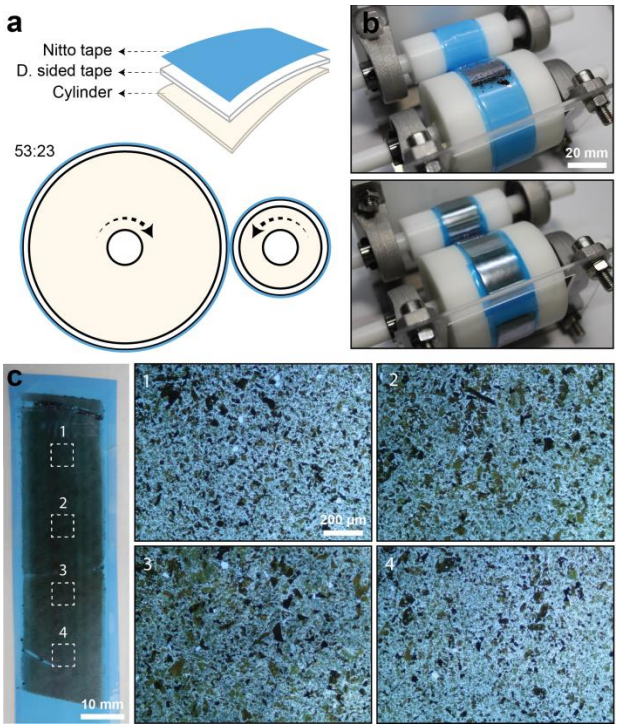

Figure 1 Massive parallel mechanical exfoliation of MoS2. a) Sketch of the massive parallel mechanical exfoliation setup. Two polyoxymethylene (POM) cylinders with incommensurate diameters (53:23) are covered with double side tape. Nitto SPV 224 tape is attached to the double side tape with its adhesive pointing outside. b) Picture of the assembled setup with a macroscopic MoS2 crystal exfoliated on the surface of one of the tapes before (top) and after (bottom) rolling the cylinders for 20 s. c) Optical image of the resulting tape after the exfoliation.

Germanene: a monoelemental 2D topological insulator

Harold J.W. Zandvliet [1,*]
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Germanene, i.e. the germanium analogue of graphene, shares many properties with graphene. Both materials host Dirac fermions, but there are also a few differences: (1) the spin-orbit coupling in germanene is much larger than in graphene and (2) the honeycomb lattice of germanene is not flat, but buckled. The large spin-orbit gap in germanene makes this material the ideal candidate to test the Kane-Mele model [1]. We show that germanene is a quantum spin Hall insulator with a gapped interior and topologically protected helical edge states [2]. The buckling of the lattice of the honeycomb allows to tailor the quantum state of matter of germanene. By applying a perpendicular electric field the spin-orbit gap in germanene first closes and then reopens again. The reopening of the gap is accompanied by a topological phase transition of germanene from a two-dimensional topological insulator to a trivial band insulator. This electric field-induced tailoring of the quantum state of matter of germanene allows to controllably switch the topologically protected helical edge states *on* and *off*. The latter makes germanene the material of choice for the realization of a topological field-effect transistor.

References

[1]. C. L. Kane and E. J. Mele**,** *Quantum spin Hall effect in graphene***,** Phys. Rev. Lett. **95**, 226801 (2005).
[2]. P. Bampoulis, C. Castenmiller, D.J. Klaassen, J. van Mil, Y. Liu, C.-C. Liu, Y. Yao, M. Ezawa, A.N. Rudenko and H.J.W. Zandvliet, *Quantum Spin Hall States and Topological Phase Transition in Germanene*, Phys. Rev. Lett. **130**, 196401 (2023).

Multi-technique study of some Xenes films: growth, structure, reactivity and optical properties

Yves Borensztein[1,*]

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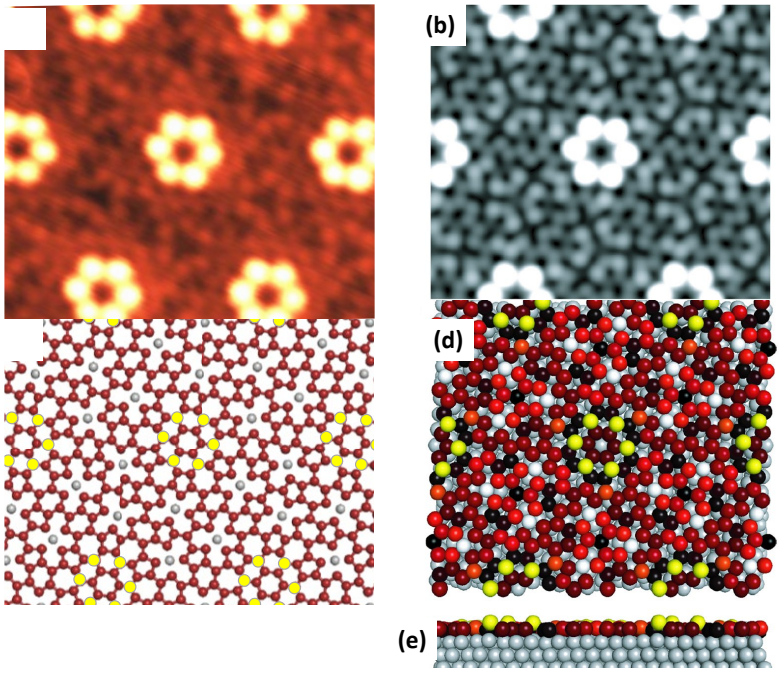
Following the advent of graphene, numerous studies have sought to obtain atomic layers of elements from column IVA of the periodic table, and monolayers of Xenes, such as silicene, graphene or stanene, have indeed been synthesized. A major difficulty is the interaction with the substrate on which these layers are formed, which can lead on the one hand to the formation of alloys and on the other hand to a modification of the electronic properties of the deposited layers compared with those expected for free-standing layers. Moreover, the resulting structures may be far from the honeycomb structure of graphene.

In this presentation, I will review the results obtained by our team over the last ten years on several systems that can lead to the formation of Xenes layers: Si on Ag, Ge on Ag and on Al, Si and Ge on HOPG. In several cases, we have elucidated the exact structures of these systems, by means of a multi-technique approach: STM, surface X-ray diffraction, optical properties, DFT and Monte-Carlo calculations...

Depending on the cases, silicene or germanene layers are indeed obtained (figure 1), while in other cases the deposited layer forms a two-layer alloy with the substrate. In particular, we have recently determined original structures: dumbbell-silicene on Ag(110), with formation of ad-atoms [1] and whose reactivity has been examined; germanene on Ag(111) formed of pentagons, hexagons and heptagons, with some Ag atoms [2].



Germanene layer grown on Ag(111). (a): experimental STM image; (c), (d) and (e): atomic structure obtained for SXRD and DFT (gray: Ag atoms ; other: Ge atoms); (b) : corresponding computed STM image [2].

References:

[1] Demonstration of the Existence of Dumbbell Silicene: A Stable Two-Dimensional Allotrope of Silicon, Leoni et al, *J. Phys. Chem. C* 2021, 125, 32, 17906

[2] The Ground State of Epitaxial Germanene on Ag(111), Zhang et al, *ACS Nano* 2023, 17, 16, 15687–15695

In-situ polarization optics in electrochemistry

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The applied electrical potential between an electrolyte and a solid electrode, whether it is a metal, semiconductor, polymer or a bio-membrane, could initiate versatile surface or film modifications. First of all, the potential simply redistribute charges. But in the new thermodynamic equilibrium adsorbates or even the conformational appearance could change and thus determine the catalytic efficiency of an electrode material, for example. From an experimental point of view, the interfacial electric potential is, on the other hand, a very precise and powerful tool to manipulate thermodynamic equilibrium conditions. It can be modified over a huge range of several eV. Similar effects are otherwise only possible with extreme e.g. temperatures or pressures. However, the fundamental knowledge about the atomic structure and the related processes is still relatively limited compared to classical surface science in vacuum. The reasons are theoretical challenges in the description but primarily experimental limitations as electron based methods like XPS are not applicable at solid-liquid interfaces. Motivated by the increasing interests in this topic, we have started to use optical polarization methods such as spectroscopic ellipsometry (SE) and reflection anisotropy spectroscopy (RAS) to obtain new and complementary in-situ information. From experiments in vacuum or gas phase environment it is known that these methods could provide an exceptional surface sensitivity. This sensitivity allows us to observe the formation of surface quantum well states at a metal-electrolyte interface or an in-situ determination of the electronic band banding at semiconductor surfaces like the polar ZnO [0001] and [000-1] surface. As a third examples we could show the electrochemical doping and formation of polarons in polymers.

Optical Spectroscopies for 2D Materials

Francesco Bisio[1,*], Ermes Peci[2], Michele Magnozzi[2], Maurizio Canepa[2]
[1]CNR-SPIN, Corso Perrone 24, 16152 Genova, Italy
[2] OPTMATLAB, Dipartimento di Fisica, Via Dodecaneso 33, 16146 Genova, Italy
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Two-dimensional materials are widely considered functional building blocks for next-generation optoelectronic devices, thanks to their striking excitonic response, strong photoluminescence yield and ultimate thinness. 2D TMDCs can be stacked on top of each other to realize van der Waals (vdW) homo- or heterostacks systems with unique properties. Interestingly, each 2D material composing the vdW stack becomes subtly influenced by the presence and the characteristics of the adjacent layers; as a result, some of its electronic properties, including the excitons, are modified with respect to the standalone case. This feature opens up the possibility to fine-tune the characteristics of each individual 2D layer by engineering its insertion within an appropriate vdW heterostructure.

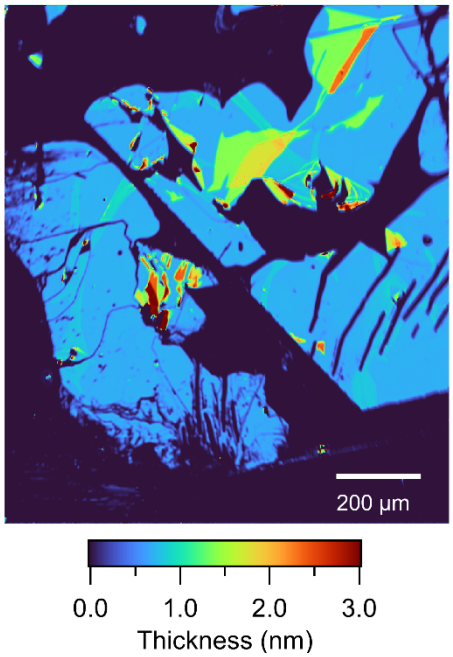

Figure 1: Thickness map of MoS_2 flakes, obtained by means of imaging spectroscopic ellipsometry.

In order to understand and characterize the response of 2D monolayers, multilayers and stacks to incoming radiation, state-of-the-art optical spectroscopy and related modelling are required.

In this contribution, I will lay the ground for the understanding of light-matter interaction, and review the application of advanced optical spectroscopies to the investigation of 2D materials. Relevant examples will deal with dimensionality effects, interlayer coupling, advanced quantitative microscopy and more [1-4].

References:

[1] Magnozzi, M. et al., "Local Optical Properties in CVD-Grown Monolayer WS2 Flakes" *Journal of Physical Chemistry C* **125**, 16059-16065 (2021)
[2] Magnozzi, M. et al., "Optical dielectric function of two-dimensional WS2 on epitaxial graphene" *2D Materials* **7**, 025024 (2020)
[3] Magnozzi M., et al., "Fast detection of water nanopockets underneath wet-transferred graphene" *Carbon* **118**, 208-214 (2017)
[4] N, Petrini et al., "Optimizing Gold-Assisted Exfoliation of Layered Transition Metal Dichalcogenides with (3- Aminopropyl)triethoxysilane (APTES): A Promising Approach for Large-Area Monolayers" Adv. Optical Mater. 2024, *in press*.

Electronic and optical properties of 2-D materials: effect of gating, twisting, and of the substrate

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We present a study of the electronic properties of 2D materials under gating, strain, stacking, doping, twisting [1]. Moire' potentials result in the opening of minigaps in the energy levels of graphene. The relative position of these minigaps is dependent on the moiré reconstruction of the system and can be tailored by tuning the rotation angle between the layers [2]. Moreover, we will discuss about the optical properties of 2-D systems. The giant excitonic effects are due to the interplay of low dimensionality, confinement effects, and reduced screening. We find exciton radiative lifetimes ranging from tenths of picoseconds (BN) to tenths of nanoseconds (InN) at room temperature, thus making 2-D nitrides [3], especially InN, promising materials for light-emitting diodes and high-performance solar cells. Finally, by using 2D modelling of the excitons [4], but also Many-Body perturbation theory approaches based on the Green's function method [5], we investigate the possibility of the existence of an excitonic insulator phase in Xenes [6].

References

[1] S. Brozzesi et al., in preparation
[2] Lifu Zhang, Ruihao Ni, and You Zhou, Journal of Applied Physics 133.8 (2023)
[3] Prete, M.S., Grassano, D., Pulci, O. et al Sci Rep. **10**, 10719 (2020)
[4] N. S. Rytova, arXiv preprint arXiv:1806.00976 (2018); L. Keldysh, Soviet Journal of Experimental and Theoretical Physics Letters 29, 658 (1979)
[5] F. Bechstedt, Many-body approach to electronic excitations (Springer Berlin, Heidelberg, 2016)
[6] O. Pulci, et al. SciPost Phys. 15, 025 (2023)

Spintronics with two dimensional materials

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The vast collection of two-dimensional materials and their co-integration in van der Waals (vdW) heterostructures enable innovative device engineering. Their atomically thin nature promotes the design of artificial quantum and topological materials by proximity-induced effects with physical properties not readily found in their single material forms. Such a flexible design approach is especially compelling for the development of spintronic devices, which usually harness functionalities from thin layers of magnetic and non-magnetic materials and their interfaces. In this tutorial I will first introduce a general review of spintronic phenomena and applications with a particular focus on 2D materials [1]. I will then summarize recent experimental progress toward investigating proximity-induced phenomena in hybrid graphene-transition metal dichalcogenides systems through spin transport dynamics and charge-spin interconversion experiments [2]. Finally, I will introduce the potential advantages of vdW heterostructures and of topological insulators (TI) for non-volatile spintronics memories [3]. Particularly, I will describe the relevance of preserving the quality of the TI/FM interfaces for the generation of highly efficient spin-orbit torques and magnetization switching in 2D ferromagnet/TI heterostructures.

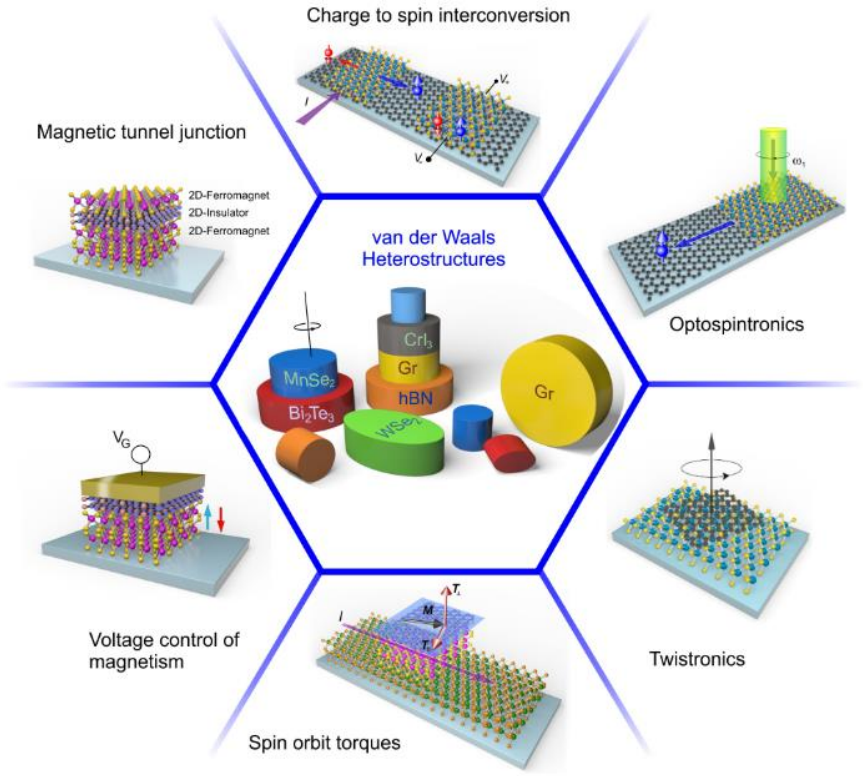

Figure adapted from Ref. [2]

References:

[1] Bernard Dieny, *et al*., *Nature Electronics* **3**, 446 (2020)
[2] Juan F. Sierra, *et al*., *Nature Nanotechnology* **16,** 856 (2021)
[3] Hyunsoo Yang, Sergio O Valenzuela, *et al*., *Nature* **606**, 663 (2022)

Photoelectronics-based on 2D materials

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The progress in spectral measurement of light is central to the advancement of scientific research and for future technologies. Spectrometers, optical devices that measure the spectral components of light, are important tools for modern applications including chemical sensing, spectral imaging, and light source characterization [1-3]. New archetype semiconductor devices utilize algorithms for driving and interpreting the I/O of photodetectors to resolve the optical spectrum. Distinct from conventional spectrometers, computational spectrometer devices necessitate bulky components or moving parts [4,5] and is based on compact semiconductor devices. Their resolution and dynamic range are subject to data sampling and electrical noise, rather than the diffraction limit of refractive optical systems. In this talk I will survey the topic of computational spectrometers and their future applications. The role of machine-learning algorithms and computational approaches will be discussed firefly as well as the importance of van der Waals materials and heterostructure devices.

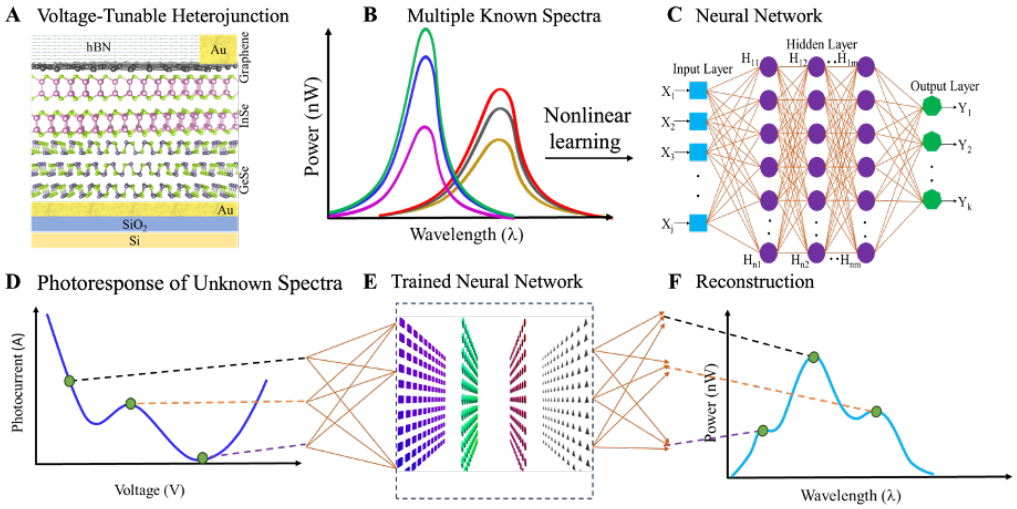

Figure 1. Illustration of a nonlinear learning and reconstruction process. (A) Schematic atomistic representation of vertical InSe/GeSe device, **(B)** that is exposed to known power-modulated spectra, **(C)** for training an artificial neural network that captures the device's nonlinear response. **(D)** A measured photocurrent vector of an unknown spectrum, (**E**) is then analyzed with the trained neural network, **(F)** enabling the reconstruction of the unknown spectrum.

References:

[1] S. Yuan et al., Nature Communications, **15**, 601-607 (2021).
[2] S. Lee et al., Nature Communications, **13**, 1485 (2022).
[3] L.Guo et al., Adv.Mater., **34**, 2200221 (2022).
[4] S. Yuan., et al. Science. **379**, 6637 (2023).
[5] Z. Ballard., et al. nature machine intelligence, **3**, 556-565 (2021).

Synchrotron-based VUV ellipsometry on passivated Si samples and Al_2O_3 for optical thin film metrology

Julian Plaickner[1,*], ,Norbert Esser[1], Alexander Gottwald[2], Mattia Mulazzi[2], Jörg Rappich[3], Karsten Hinrichs[4], Christoph Cobet[5], Jakob Zessin[6], Johanna Reck[6], Uwe Richter[6]

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Optical reference materials were measured in the vacuum ultraviolet (VUV) spectral range (between 3 and 30 eV) with synchrotron-based ellipsometry. This spectral range is characterized by a lack of reliable data on optical properties due to the extreme surface sensitivity and the requirements of a high brightness light source. The synchrotron-based VUV ellipsometer[1] at the Metrology Light Source (MLS) and numerical modeling in a hybrid metrology approach are used for a reference-free determination of the optical properties. The developed methods are tested on substrates with well-defined surface structures, i.e. on chemically-passivated vicinal silicon substrates with variable step density. In particular, ellipsometry results on CH_3-passivated Si surfaces and ALD-prepared Al_2O_3 samples were shown and a model for the determination of statistical and systematic uncertainties is provided. X-ray photoelectron spectroscopy (XPS) and IR ellipsometry measurements serve as quality cross checks for the prepared surfaces. In the spectral range between 2 and 6 eV, results are compared to reference measurements made with commercial SENTECH ellipsometers. The financial support by the European Union through EFRE 1.8/13 and ProFIT OptiRefS (Nr. 10185437) is acknowledged.

References:

[1] M. D. Neumann et al., Rev. Sci. Instrum. 85, 055117 (2014)

Roll-to-Roll Exfoliation for Anisotropic Films of 2D Materials

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The recent development of roll-to-roll high-throughput exfoliation technique for the production of high-density van der Waals materials has opened a world of possibilities for scaling the fabrication of electronic devices based on 2D materials[1]. This method has shown to produce large-area films composed of interconnected flakes of van der Waals materials, yielding superior device performance compared to other low-cost, high-yield 2D material production methods like liquid-phase exfoliation In addition to its scalability, we have explored the potential of leveraging the unidirectional exfoliation orientation that this method offers to exfoliate materials with highly anisotropic structures, such as black phosphorus (BP) or germanium sulfide. Since this exfoliation method tends to preserve the orientation of our materials, we are able to fabricate polarizers or photodetectors that respond based on the incident light angle.

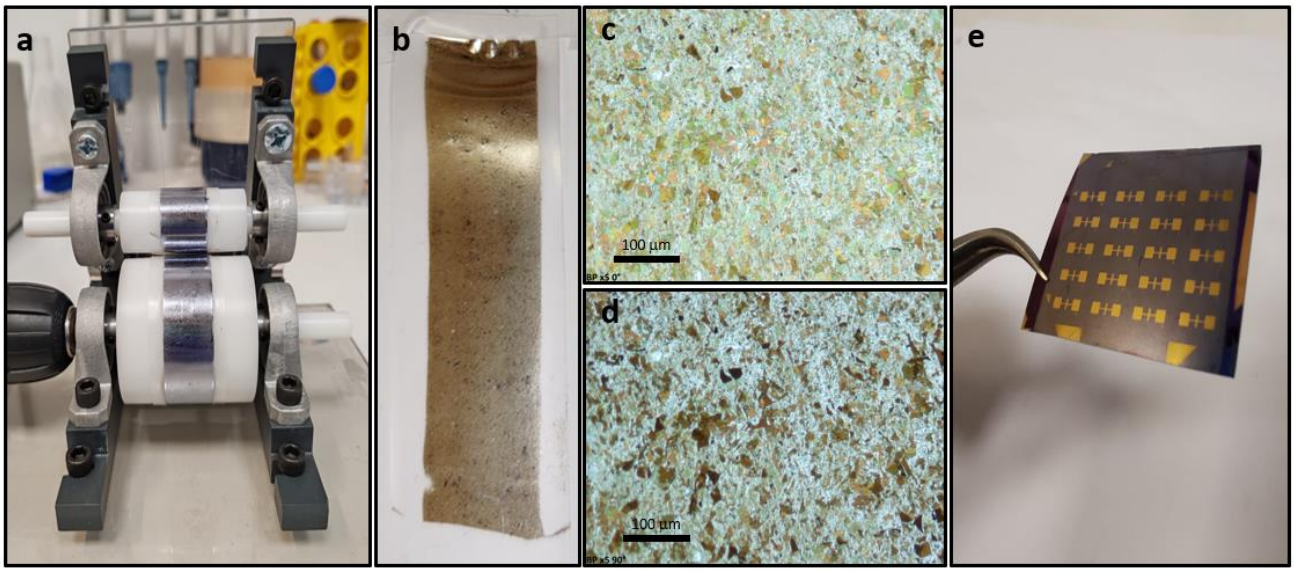

Figure 1 a) Picture of the massive parallel exfoliation device after the exfoliation of the crystal of BP. b) Picture of the sample obtained after exfoliation. c) Picture of the tape under the microscope, illuminated with light polarized at a 0-degree angle. d) Picture of the tape under the microscope, illuminated with light polarized at a 90-degree angle. e) Fabrication of devices on a silicon oxide wafer by thermal evaporation to analyze their optical and electrical properties.

References:

1. Sozen, Y., Riquelme, J. J., Xie, Y., Munuera, C. & Castellanos-Gomez, A. High-Throughput Mechanical Exfoliation for Low-Cost Production of van der Waals Nanosheets (Small Methods 10/2023). *Small Methods* **7**, (2023).

Nanopatterning 2D semiconducting layers for large-scale photon harvesting and nanoelectronics

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Two-dimensional (2D) Transition Metal Dichalcogenide semiconductors (TMDs) have attracted strong interest due to their exceptional optoelectronic properties [1,2]. However, the inherent low photon absorption of the atomic layers demands for novel light coupling schemes. There is also an urgent request to scale-up the lateral size of the 2D layers, so far limited to micrometer scale flakes, and to engineer their shape at the nanoscale. [3]. Here we address such issues , focusing on large area physical deposition of TMD semiconductors, and on flat-optics photon harvesting schemes. Few-layers TMD films are nanopatterned as periodic nanogratings which support narrowband Rayleigh anomalies as well as brodband guided modes. Strong in-plane light confinement thus boosts photon absorption in the ultra-thin layers [4,5].
More complex TMD heterostructure architectures (MoS2/WS2) can also be obtained by combining large are physical deposition of TMD layers, with maskless and self-organised nanofabrication by sequential glancing angle shadow epitaxy on a periodically nanotextured templates. These results show that large area arrays of TMDs van der Waals heterostructures with type-II band alignment can represent a viable approach towards real-world applications of 2D-TMD devices in self-powered photoconversion applications (photocatalysis, electro-optical conversion etc) [6].
A substantial advancement is represented by the possibility of fabricating arbitrarily defined few-layer MoS2 nanopaths and nancircuits thanks to a new additive nanofabrication approach, based on a combination of thermal-Scanning Probe Lithography with large area physical deposition of TMDs by ion beam sputtering, showing the potential of these building blocks in ultra-thin integrated electronic and photonic devices. A further degree of freedom which enables light harvesting is given by the combination of TMD materials with plasmonic nanostructures
The combination of large-scale nanopatterning approaches with non-invasive 2D-TMD thermal lithograpy thus open new promising possibilities for the integration of 2D TMDs layers in scalable opto-electronic and energy conversion applications.

References

[1] C. Martella, et al. Advanced Materials, 30 (9), 1705615, 2018.
[2] C. Martella, et al. Advanced Materials 29 (19), 1605785, 2017.
[3] C. Mennucci et al. Advanced Optical Materials 9 (2), 2001408, 2021.
[4] C. Bhatnagar, et al. Nanoscale 12 (48), 24385, 2020.
[5] M. Bhatnagar, et al. ACS Applied Materials & Interfaces 13 (11), 13508, 2021.
[6] M. Gardella et al., RSC Appl. Interfaces, 2024 Advance Article DOI: 10.1039/D3LF00220A
[7] M.C. Giordano, et al. Adv. Mater. Interfaces 10, 2201408, 2023.

Room Temperature Superfluorescence in Perovskites and Its Implications for Quantum Materials

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The formation of coherent macroscopic states and the manipulation of their entanglement using external stimuli are essential for emerging quantum applications. However, the observation of collective quantum phenomena such as Bose–Einstein condensation, superconductivity, superfluidity and superradiance has been limited to extremely low temperatures to suppress dephasing due to random thermal agitations. In this presentation we will talk about room-temperature superfluorescence (SF) in hybrid perovskite thin films [1,2]. In SF an optically excited population of incoherent dipoles develops collective coherence spontaneously. This emergent collective state forms a giant dipole and radiates a burst of photons [Fig. 1]. Because electronic transitions dephase extremely fast, observation of SF in semiconductors is extremely rare and under high magnetic fields and at very low temperatures [3]. Therefore, the discovery of room temperature SF in perovskites is very surprising and shows that in this material platform, there exists an extremely strong immunity to electronic dephasing due to thermal processes. To explain this observation, we propose that the formation of large polarons in hybrid perovskites provides a quantum analogue of vibration isolation to electronic excitation and protects it against dephasing even at room temperature. Understanding the origins of sustained quantum coherence and the superfluorescence phase transition at high temperatures can provide guidance to design systems for emerging quantum information technologies and to realize similar high-temperature macroscopic quantum phenomena in tailored materials.

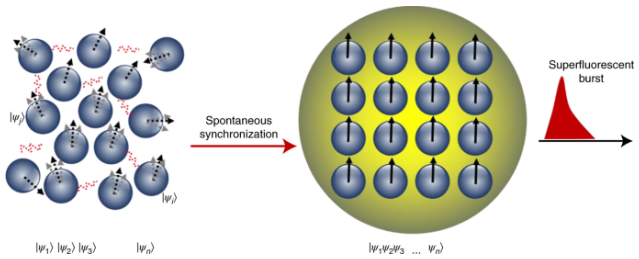

Figure 1 An incoherent ensemble of dipoles is shown on the left. Arrows indicate the randomly distributed phases of individual dipoles. The red waves resemble vacuum fluctuations, which lead to spontaneous synchronization. After a time delay, the phases of the excited dipoles are locked, forming a macroscopic quantum coherent state: a 'giant atom' (on the right). The collective emission of the macroscopic coherent system leads to a superfluorescent burst.

References

[1] M. Biliroglu et.al., Nature Photonics **16**, pages324–329 (2022)
[2] G. Findik et.al., Nature Photonics **15**, pages 676–680 (2021)
[3] G. Timothy et.al., Nature Physics **8**, pages219–224 (2012)
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Homogenization of multicomponent metamaterials

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The use of inhomogeneous artificial media such as metamaterials and photonic crystals made up of alternating particles of diverse ordinary materials have led to novel optical devices, sometimes with exotic properties. One approach to their calculation is *homogenization*, i.e., replacing the position dependent dielectric function $\varepsilon(\mathbf{r})$ of the composite, with different values within each one of its components, by a single homogeneous effective dielectric tensor $\boldsymbol{\varepsilon}_M$. In this work we extend an efficient homogenization procedure [1] based on Haydock's recursive procedure [2] to obtain $\boldsymbol{\varepsilon}_M$ for a system made of an arbitrary number of materials, allowing for their possible dispersion, dissipation and anisotropy. The homogenized response is in general spatially dispersive $\boldsymbol{\varepsilon}_M(\mathbf{k},\omega)$, indicative of optical activity and magnetic properties [3]. We test our formalism applying it to a helicoidal Bouligand structure [4] such as that in the iridescent cuticles of some insects. From the macroscopic response we obtained the photonic bands $k(\omega)$, with gaps for only one helicity, explaining the circular polarization observed in reflection spectra. We confirmed the numerical results by comparison with an analytical model and applied them to other multicomponent systems.

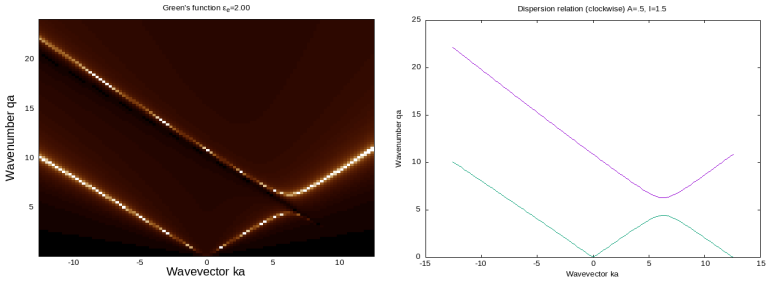

Figure 1 Numerical (left) and analytical (right) dispersion relation of a circular polarized mode propagating along a Bouligand structure.

References:

[1] W L Mochán et al., https://doi.org/10.1364/OE.18.022119 Opt. Express **18** 22119 (2010).
[2] R Haydock, Sol. St. Phys. **35** 215 (1980).
[3] L Juárez-Reyes and W L Mochán https://doi.org/10.1002/pssb.201700495 Physica Status Solidi (b) **255** 1700495 (2018).
[4] Y Bouligand https://doi.org/https://doi.org/10.1016/S0040-8166(72)80042-9 Tissue and Cell **4** 189 (1972).

Optical properties of metallic nanowires

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One-dimensional structures where two dimensions are in the nanometer scale and thus smaller than the wavelength of light have a wealth of interesting optical properties. *Metallic* NWs give the possibility of exciting size and shape dependent plasmon resonances, adding to the scattering properties. Some examples of applications of metallic NWs are presented.

Spectrally selective absorption and scattering have exciting applications in solar energy technology. Thin film solar cells have limited efficiency due to the poor absorption in Si. By scattering light above the critical angle in Si by horizontally oriented NWs, a substantially higher fraction of the incident light is captured inside the Si film. Vertically oriented NWs, on the other hand, supports gap plasmons that lead to strong absorption of the incoming field. Examples of applications as absorbers and emitters in thermophotovoltaics, using TiN as plasmonic material, are presented.

Surface enhanced Raman spectroscopy takes advantage of plasmonic effects generating large local fields in the gaps between NWs. Orders of magnitude enhancement of the Raman detection limit is demonstrated with glancing angle deposited Au and Ag films [1].

The 1D symmetry of NWs has a strong impact on second-order nonlinear optics and introduce new effects, for instance in second harmonic generation. GLAD NW samples are intrinsically achiral, i.e. they have a plane of mirror symmetry. However, chirality is demonstrated in SHG from such surfaces, caused by the combined substrate symmetry and the geometry of the optical experiment. (Figure 1).

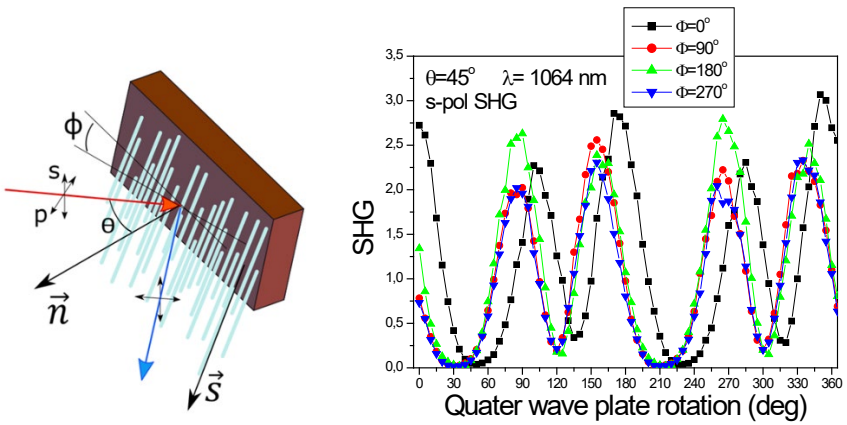

Figure 1 a) NW orientation and laser beam direction. b) SHG as a function of the rotational angle of a quarter-wave plate in the incident laser beam recorded for 4 different sample orientations.

References:

1. [1] A. Chirumamilla et al, Applied Materials Today, **31**, 101763 (2023).

Optical Nanospectroscopy for Tissue Imaging and Early Cancer Diagnostics

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Keywords: (Raman, SNOM, IR, Cancer Cells, ALS)

Carcinomas are complex biochemical systems and in the past their diagnosis was based on morphological differences between malignant cells and their benign counterpart. Recently the paradigm has changed and great interest is focused now on the biochemical profile of tumours in view of the availability of new drugs that specifically target neoplastic cells. This new paradigm requires biochemical analysis of each tumour in order to establish the correct personalized oncological "target therapy". Understanding the mechanism of molecular alterations of a specific tumour is a critical issue to predict the response to personalized therapy. This is important not only for discrimination between healthy and pathological tissues, but also for pre-cancerous tissue state earlier detection and understanding.
The potential of infrared [1] and Raman spectroscopy [2] to characterise cancerous tissues has long been recognised and studies of various cancers by many groups have established that regions of malignant tissue can be easily identified on the basis of its optical spectrum. Early diagnosis of cancer requires an instrument providing specific chemical images at sub-cellular level and the development of diagnostic imaging. Infrared Scanning Near-field Optical Microscopy (IR-SNOM) and micro-Raman set-up meet these requirements provided that SNOM can been coupled with an appropriate infrared light source, that can be based on Free Electron Laser, femtosecond laser or quantum cascade laser.
We present IR-SNOM and micro-Raman in their spectroscopic mode, that is related to the local chemical composition and, thus, to the biological properties of the sample, for tissue imaging and early cancer diagnostics. Applications in the case of Oesophagous [3] and Cervical Cancer [4] as well as in the progression of Amyotrophic Lateral Sclerosis (ALS) will be presented.

[1] Cricenti A, Luce M, Tolk NH, Margaritondo G; Nanosci. Nanotechnol. Lett.; 3 (2011) 913;
[2] Çulha M, Bioanalysis, **7**, 2813 (2015)
[3] Smith AD, Siggel-King MRF, Holder GM, Cricenti A, Luce M, Harrison P, Martin DS, Surman M, Craig T, Barrett SD, Wolski A, Dunning DJ, Thompson NR, Saveliev Y, Pritchard DM, Varro A, Chattopadhyay S, Weightman P; Applied Physics Letters; 102 (2013) 053701.
[4] Halliwell Diane E, Morais Camilo LM, Lima Kássio MG, Trevisan Julio, Siggel-King Michele RF, Craig Tim, Ingham James, Martin David S, Heys Kelly A, Kyrgiou Maria, Mitra Anita, Paraskevaidis Evangelos, Theophilou Georgios, Martin-Hirsch Pierre L, Cricenti Antonio, Luce Marco, Weightman Peter, Martin Francis L; Nature Scientific Reports; 6 (2016) 29494.

Overview on 2D Material-based Inks: from Fundamentals of Colloidal Chemistry to Applications

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After the discovery of graphene in 2004, the field of atomically thin crystals has exploded with the discovery of thousands of 2-Dimensional materials (2DMs) with unique electronic and optical properties, hence making 2DMs very attractive for a broad range of applications - from electronics to energy storage and harvesting, and from sensing to biomedical applications. Furthermore, 2DMs can be easily produced in solution, hence enabling the use of mass scalable and low cost techniques, such as inkjet printing, for the integration of 2DMs into devices onto flexible substrates, such as paper and plastic [1].

In this tutorial, I will first discuss the fundamentals of colloidal and interface chemistry [2], which will be then applied to the production of stable and concentrated dispersions of 2D materials in water. I will discuss the different approaches used in literature with a particular focus on the use of non-covalent functionalization using pyrene derivatives [3]. I will discuss the different printing technologies and describe the properties of printed films made of nanosheets. Finally, I will discuss a couple of examples of printed devices made of 2DM-based inks.

References:

[1] Conti et al, Nature Reviews Materials 8 (10), 651-667 (2023)
[2] Introduction to Colloid and Surface Chemistry, Duncan Shaw, Elsevier
[3] Hu et al, Nanoscale, Nanoscale 13 (2), 460-484 (2021)

Fabrication of van der Walls stacks

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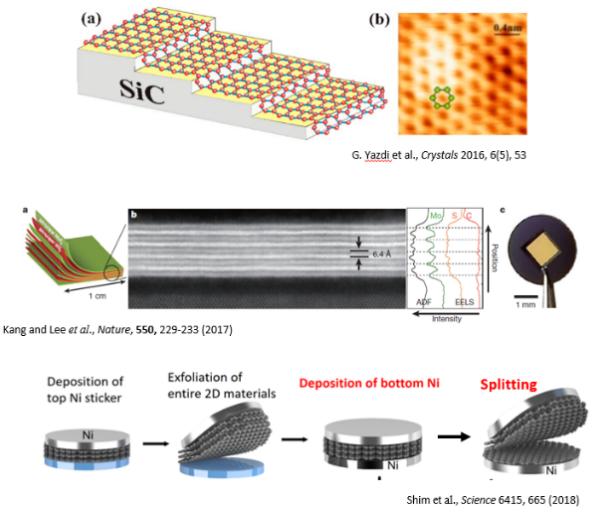
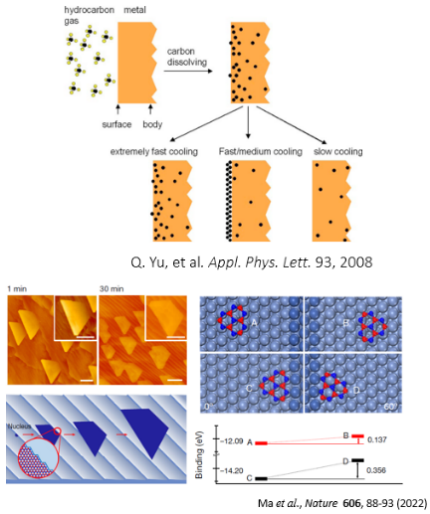
Van der Waals (vdW) materials represent a unique class of substances held together by weak interlayer forces known as van der Waals forces. These materials typically consist of atomically thin layers, such as graphene, transition metal dichalcogenides (TMDs) like MoS2 and WSe2, and hexagonal boron nitride (h-BN), collectively referred to as 2D materials. These layers can be easily exfoliated due to the weak interlayer forces, enabling the isolation of individual atomic layers.

Moreover, vdW stacks, also known as layered heterostructures, are formed by stacking these individual layers on top of each other. The weak van der Waals forces between layers allow for the assembly of these atomically thin layers into three-dimensional structures, providing new device architectures and platforms for interesting physical coupling. Recently, the development of freestanding 3D nanomembranes has introduced a new avenue for creating vdW stacks, combining 2D materials with 3D nanomembranes. This hybrid approach overcomes the limitations of traditional 2D material-based vdW stacks, which are restricted by the number of atoms in the layers, by incorporating the structural diversity of 3D nanomembranes.
In this discussion, I aim to explore various methodologies for producing both 2D materials and 3D nanomembranes, which serve as the fundamental building blocks for constructing vdW stacks. I will introduce the historical evolution of growth techniques for 2D materials, including sublimation-based growth, catalytic growth, kinetic-control-based growth, epitaxial growth, and non-epitaxial growth. Additionally, I will examine various layer transfer techniques to fabricate single-crystal 3D nanomembranes, providing insights into the versatile methods used to engineer these materials.





References:

[1] G. Yazdi et al., *Crystals* 6(5), 53 (2016), [2] Kang *et al*., *Nature*, **550,** 229-233 (2017), [3] Shim et al., *Science* 6415, 665 (2018), [4] Q. Yu, et al. *Appl. Phys. Lett.* 93, 2008, [5] Ma *et al*., *Nature* **606**, 88-93 (2022)

Tunable Second Harmonic Generation in 2D Materials from First-Principles

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Non-linear optical frequency conversion, where optical fields interact with a non-linear medium to generate new field frequencies, is widespread in modern photonic systems. However the challenging aspect often lies in tuning the non-linear electrical susceptibilities responsible for such phenomena in a specific material. Consequently, the dynamic control of optical non-linearities, utilized as a spectroscopic tool, has, until now, mainly been confined to research laboratories. From an experimental point of view, different experiments have revealed the possibility of using external fields to induce and modify SHG in 2D materials [1-4]. In this work we explore a mechanism for electrically manipulating second-order optical non-linearity in two-dimensional materials. In particular, we will consider a 2 layers system (2H-MoS2), which presents a zero second harmonic generation (SHG) due to spatial inversion symmetry. By using an ab initio real-time approach [5], developed within the Yambo code [6], we show how the effect of an external vertical electric field can induce and modify an SHG response and the role of bound excitons in this non-linear response.

References:

[1] J. Klein, et al., Nano Letters 17(1), 392 (2017).
[2] S. Shree, et al., Nat. Comm. 12(1), 6894 (2021).
[3] J. Wang, et al., ACS Nano 16(4), 6404 (2022).
[4] K. L. Seyler, et al., Nat. Nanotechnol. 10(5), 407 (2015).
[5] C. Attaccalite and M. Gruning, Phys. Rev. B. 88(23), 235113 (2013).
[6] D. Sangalli, et al., J. of Phys.: Cond. Matt. 31(32), 325902 (2019).

Analysis of the Absorption Resonances between Carbynes and Cyclo[*n*]carbons: a tight-binding approach

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We present a different method of solving an old problem of molecular rings and chains [1] with one-to-one correspondence as an initial step to analyzing the electronic and optical properties of *sp*-hybridized carbon allotropes. By implementing the transfer matrix method within the analytical tight-binding method, the eigenenergies of an atomic ring such as a cyclo[*n*]carbon match the eigenstates of a finite chain, a cumulenic carbyne, when the number of atoms in a ring is twice the number of atoms with an additional of two atoms, i.e., $N_{ring} = 2N_{chain} + 2$ as shown in Figure 1. Our results agree with the geometrical projection scheme of one-to-one relation in energies of atomic rings and finite chains [1,2]. However, it does not immediately imply a correlation in their optical absorption due to the different selection rules [3]. Here, we show that both an atomic ring and a finite chain can have similar optical transitions between eigenstates *n* and *m* when the eigenstates difference is +/-1. Compared to the atomic rings, the corresponding finite chains have more transitions between eigenstates with odd differences (+/-3,+/-5, …). However, the magnitude of higher-order transitions drastically diminishes as the odd differences between eigenstates increase. Thus, the absorption spectra of an atomic ring can be correlated to the finite atomic chain when their energy levels match.

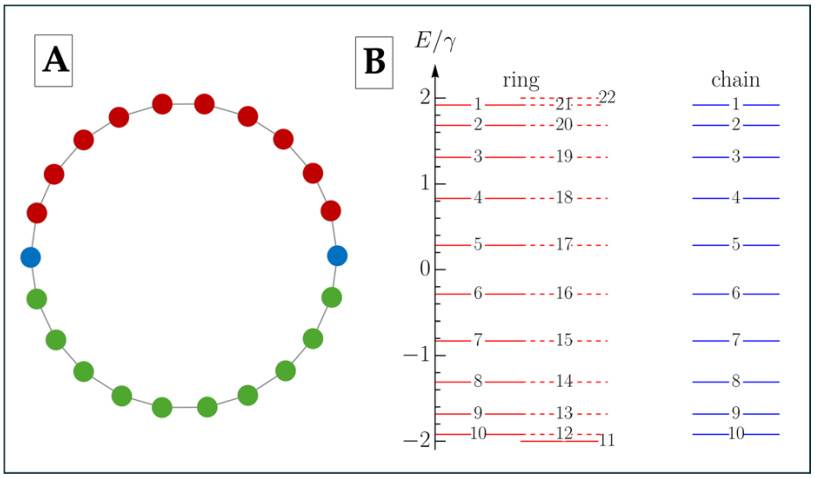

Figure 1 A. The decomposition of atomic ring $N_{ring} = 22$ into two chains $N_{chain} = 10$ (red, green) with their (B) equivalent energy levels. The two extra atomic sites (blue) together with the two chains complete an atomic ring structure, which represents the 2N + 2 – rule decomposition. All eigenenergies of the finite atomic chain $N_{chain} = 10$ match the corresponding double degeneracies of an atomic ring $N_{ring} = 22$, except at the atomic ring boundary points +/-2.

References:

[1] Frost, A.A., Musulin, B., "A mnemonic device for molecular orbital energies," The Journal of Chemical Physics **21**, 572-573 (1953).
[2] E. Hückel, "Quantentheoretische beiträge zum problem der aromatischen und ungesättigten verbindungen III" Zeitschrift für Physik **76**, 628–648 (1932).
[3] R. B. Payod, D. Grassano, G. N. C. Santos, D. I. Levshov, O. Pulci, and V. A. Saroka, "2n+ 4-rule and an atlas of bulk optical resonances of zigzag 48graphene nanoribbons," Nature communications **11**, 1–9 (2020).

Experimental observations of the acoustic surface plasmon: from Electron Energy Loss Spectroscopy to Hyperthermal atom scattering.

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Acoustic surface plasmon are typically observed when a 2D and a 3D electron gas coexist.
Indeed, while for a purely two dimensional system collective electronic excitations exhibit a square root dispersion, in presence of a three dimensional electron gas the counter phase motion of 2D and 3D electrons gives rise to a novel collective excitation, the Acoustic Surface Plasmon (ASP).
The ASP is characterized by a linear dispersion and by a vanishing energy in the long wavelength limit.
The existence of the ASP was firstly predicted theoretically [1]; this talk reviews the experimental observations of the Acoustic Surface Plasmon [2], starting from its first observation on Be(0001) by High Resolution Electron Energy Loss Spectroscopy [3], to its observation by hyperthermal neon scattering off Cu(111) [4]. Indeed, since its energy falls in the sub-eV region the ASP represents a so

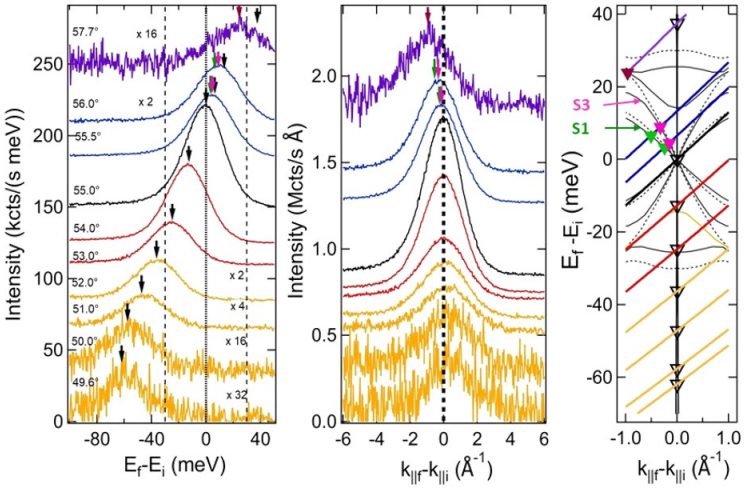

Figure 1. Spectra as a function of kinetic energy difference (left) and of parallel momentum (center) as well as for different θ_i. The right panel shows the relevant scan curves and the nearly vertical dispersion. (From ref. [4]).

far neglected channel for energy dissipation in gas- surface scattering and can have a non-negligible probability of thermal excitation.

References:

[1] J.M. Pitarke, V.M. Silkin, E.V. Chulkov and P.M. Echenique, Theory of surface plasmons and surface-plasmon polaritons, *Rep. Prog. Phys*. **70**, 1 (2007)
[2] H. Pfnuer, C. Tegenkamp and L. Vattuone, in Plasmons in One and Two dimensions, Springer Handbook of Surface Science, editors M.Rocca, T.S. Rahman and L. Vattuone, chap. **19**, 561 (2021)
[3] B. Diaconescu, .., L. Vattuone, et al., Low-energy acoustic plasmons at metal surfaces, *Nature*, **448**, 57 (2007)
[4] G. Bracco, L. Vattuone, .., G. Benedek et al., Prominence of acoustic surface plasmons in hyperthermal gas energy transfer to metal surfaces, *J. Phys. Chem. Lett.* **12**, 9894 (2021)

Proximity coupling effects in epitaxial 2D graphene-based systems

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Currently, 2D materials and their heterostacks of 2D materials are in the focus of research and are expected to be building blocks for new quantum materials. Therefore, proximity coupling is in general a very important concept. Epitaxial graphene (EG) grown on SiC(0001) resembles a truly 2D electron gas system and is known for its ability of manifold and flexible functionalization schemes at its vacuum and interface site. These functionalization schemes allow to realize extreme doping scenarios in graphene, tune the spin-orbit coupling, realize interface states and introduce mini-bands by zone folding. The controlled transition from linear to flat bands in EG as well as the coupling of functionalized graphene to 2DEGs will open the corridor for electronic correlation effects and mesoscopic phenomena in 2D materials, e.g. superconductivity, charge and spin density waves, Mott states, etc.

In this talk I will highlight some recent experiments towards the coupling of epitaxial Bi islands on monolayer graphene as well as the intercalation of Pb below graphene. Upon adsorption, epitaxial Bi(110) islands are formed, which change the initial n-type doping of MLG locally [1]. The formation of inhomogeneous carrier concentration profiles on MLG results in a positive and linear magnetoresistivity effect with increasing Bi coverage. By extracting the carrier concentration from the Shubnikov-de Haas oscillations, we confirm that the carrier concentration in the uncovered regions remains constant. Moreover, the signatures of weak localization in the magnetoresistivity vanished with increasing Bi coverage, while no signs of weak anti-localization were found at all. Apparently, the proximitized Bi islands induce a well-defined lateral doping profile so that the electrons are not penetrating into the areas of the Bi-islands, thus mimicking antidots.

Regarding intercalation of buffer layer structures on SiC(0001), intercalated Pb bilayers form nanostripes under graphene and show fingerprints of plumbene. These Pb layers are rotated with respect to graphene, which breaks the sublattice symmetry and is associated with an electronic gap in graphene [1]. Intercalated Pb monolayer show a defined grain boundary network and efficiently minimizes the doping influence by the SiC substrate, giving rise to charge-neutral monolayer graphene. *[2]. T*he conductivity decreases with decreasing temperature down to 30 K, revealing clearly a non-metallic behavior. We address the finding to a small gap opening (1-5 meV) in graphene via the proximitized 2D Pb layer, e.g. spin orbit coupling in graphene.

The adsorption of 1/3 ML of Sn on SiC(0001) was shown to reveal a robust 2D Mott state. We studied the electronic structure of intercalated Sn below the buffer layer on SiC(0001) coming along with the formation of n-type doped graphene. By means of EELS and STS we analyzed in detail the electronic structure and found strong evidence of a hybridization between Sn-induced Mott states and the graphene π-bands. This leads to a gap opening of around 200 meV at the Dirac point. Moreover, a new state at around 1.2 eV emerged which we assign to the upper Hubbard band. The formation of narrow bands is supported by EELS measurements, showing besides the sheet plasmon also a pronounced interband transition at 1.5 eV. Combined DFT and dynamical mean field theory calculations support the emergence of strong Mott Hubbard correlations in this system.

References:

[1] J. Koch et al. Journal of Physics: Condensed Matter, 36, 065701 (2024)
[2] C. Ghosal et al., Phys. Rev. Lett. 129, 116802 (2022)
[3] P. Schädlich et al. Adv. Mat. Int. 10, 2300471 (2023)

Low-energy collective electronic excitations at metal surfaces and layered materials

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In the heterogeneous systems the collective electronic excitations, called plasmons, can be very different of the conventional plasmon in bulk. This can be explained by differences of the electronic band structure of real materials from the idealized free-electron gas (FEG) behavior. Thus, a variety of metal surfaces such as (111) surfaces of noble metals Cu, Ag, and Au, and Be(0001) are known to support a partially occupied electron bands of the Shockley surface state at the center of the surface Brillouin zone. This state has a parabolic-like dispersion with two-dimensional (2D) momentum, $\mathbf{q}_{\|}$, parallel to the surface and their wave functions are strongly localized near the surface. Indeed, these surface states are immersed in the sea of bulk electrons and the charge corresponding to surface states constitutes only small fraction of total electronic charge at metal surfaces. However, due to its 2D character this surface state can strongly modify the dielectric properties of surfaces. Some time ago is was demonstrated [1] that due to the coexistence of carries near a metal surface in bulk and surface bands there is a possibility for existence of a novel kind of collective electronic excitations – acoustic surface plasmon (ASP). Such modes were observed on several metal surfaces [2,3] and graphene-based systems. In the layered bulk materials existence of a similar mode, called acoustic plasmon (AP), was predicted in a number of *ab initio* calculations. Very recently it was announced on its experimental detection in Sr_2RuO_4 [4], although the measured AP dispersion was very different of the calculated one.

An interesting property of the ASP and AP is a quasi-linear sound-like dispersion with momentum **q**, for small values of q, different to the $\sqrt{q}$ behavior to a 2D plasmon. The slope of its dispersion is determined by the Fermi velocity of the carriers in the slowest band. Usually, it is implicitly assumed that a multi-component electronic system, need for realization of ASP and AP, can be realized when several energy bands cross the Fermi level. However, recently it was demonstrated [5] that an acoustic mode can exist, in addition to the conventional plasmon, in a *single* energy band with a dispersion strongly deviating from the FEG isotropic case. Thus, the effect of the anisotropy of the energy band may not be limited to the change of the conventional plasmon dispersion only, but can led to the appearance at lower energies of additional acoustic modes in certain symmetry directions. Moreover, the in some systems effect of the energy dispersion may be even more dramatic. For instance, it was predicted that in the optimally doped cuprate superconductors in the normal state, peculiar modes with sound- and one-dimensional-like dispersions can exist as well [6].

In present contribution the properties of all these low-energy electronic modes will be discussed.

References:

[1] V. M. Silkin et al., Europhys. Lett. **66**, 260 (2004).
[2] B. Diaconescu et al., Nature **448**, 57 (2007).
[3] L. Vattuone et al., Phys. Rev. Lett. **110**, 127405 (2013).
[4] A. A. Hussain et al., Nature **621**, 66 (2023).
[5] U. Muniain and V. M. Silkin, Phys. Chem. Chem. Phys. **24**, 17885 (2022).
[6] V. M. Silkin, S.-L. Drechsler, D. V. Efremov, J. Phys. Chem. Lett. **14**, 8060 (2023).

Strain engineering of 2D materials

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2D semiconductors are very appealing because of their optoelectronic properties. The combination between these optoelectronic properties and their unique mechanical properties provides a powerful strategy to tune the functional properties through the deformation of these materials.

Traditional methods of straining 3D materials, such as epitaxial growth on mismatched substrates, are often restricted to strains below 2% due to the inherent brittleness of bulk semiconductors. For instance, bulk silicon can only withstand strains up to 1.5% before failure. Moreover, these methods typically induce static deformations, rendering them unsuitable for dynamically tunable devices.
The outstanding stretchability of 2D materials [1] (and the possibility of using dynamically varying strain) holds the promise of revolutionizing the field of strain engineering and could lead to "straintronic" devices – devices with electronic and optical properties that are engineered through the introduction of mechanical deformations.
In this tutorial I will discuss the different strategies developed to study strain engineering in 2D materials and to exploit it to fabricate strain tunable functional optoelectronic devices [2-8].

[1] R Roldán et al. Journal of Physics: Condensed Matter (2015) 27 (31), 313201
[2] H. J. Conley et al. Nano Lett. (2013) 13, 3626
[3] K. He et al. Nano Lett. (2013) 13, 2931
[4] A Castellanos-Gomez, et al. Nano letters (2013) 13 (11), 5361-5366
[5] J Quereda, et al. Nano letters (2016) 16 (5), 2931-2937
[6] JO Island, et al. Nanoscale (2016) 8 (5), 2589-2593
[7] R Schmidt et al. 2D Materials (2016) 3 (2), 021011
[8] R Frisenda, et al. npj 2D Materials and Applications (2017) 1 (1), 10

Self-consistent Hubbard parameters in doped layered transition-metal oxides for sodium-ion batteries

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Sodium-ion batteries share similarities with the well-established lithium-ion batteries currently in widespread use [1]; in fact, analogously to lithium-ion positive electrodes, sodium-ion cathodes store sodium through an intercalation mechanism. Cathodes based on P2-Na_xTMO_2 crystals, i.e., sodium-based layered transition-metal oxides (LTMOs), have attracted growing interest owing to their high potential and capacity [2]. However, the geometric structure of LTMOs may undergo a Jahn-Teller distortion during charge/discharge cycles. Doping has proven effective in stabilizing the P2 geometric structure improving the cycling stability by limiting structural transitions as well as delaying them at higher voltages. Ab-initio calculations within the Quantum ESPRESSO suite [3] are employed to determine the optimal dopants, the total energy of the system, and estimate the sodium-ion intercalation potential. The structural and electronic properties of doped LTMOs are investigated at a GGA + *U* level of theory, where the on-site Hubbard *U* parameters are evaluated self-consistently using linear-response theory [4], so to realistically include the screening from the environment which is crucial for quantitatively predictive calculations.

References

[1] Kim, S. W., Seo, D. H., Ma, X., Ceder, G., & Kang, K. (2012). Electrode materials for rechargeable sodium-ion batteries: potential alternatives to current lithium-ion batteries. *Advanced Energy Materials*, *2(7)*, 710-721.

[2] Clément, R. J., Bruce, P. G., & Grey, C. P. (2015). manganese-based P2-type transition metal oxides as sodium-ion battery cathode materials. *Journal of The Electrochemical Society*, *162(14)*, A2589.

[3] Giannozzi, P., Baroni, S., Bonini, N., Calandra, M., Car, R., Cavazzoni, C., ... & Wentzcovitch, R. M. (2009). QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. *Journal of physics: Condensed matter*, *21(39)*, 395502.

[4] Cococcioni, M., & De Gironcoli, S. (2005). Linear response approach to the calculation of the effective interaction parameters in the LDA+ U method. *Physical Review B*, *71(3)*, 035105.

Growth of group 14 elemental post-graphene materials

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The synthesis and characterization of post-graphene materials have been intensively studied with the aim of utilizing novel two-dimensional (2D) properties. Most studies adopted molecular beam epitaxy as a synthesis method of 2D materials grown on clean crystalline surfaces. In my talk, I will talk on the epitaxial growth of (1) germanene, (2) stanene, lateral heterostructure, and (3) plumbene by segregation and deposition methods [1–11].

(1) Germanene on Ag(111) thin film by segregation [1]: On annealing the specimen of Ag(111) thin film grown on Ge(111)the Ge atoms segregate on the surface and germanene has been epitaxially formed on the surface. Low-energy electron diffraction clearly shows incommensurate "(1.3×1.3)"±30° spots, corresponding to a lattice constant of 0.39 nm, in perfect accord with close-up scanning tunneling microscopy (STM) images, which clearly reveal an internal honeycomb arrangement with corresponding parameter and low buckling within 0.01 nm. From the STM images, two types of protrusions, named hexagon and line, form a $(7\sqrt{7}\times7\sqrt{7})$ ±19.1° supercell with respect to Ag(111) with a super large periodicity of 5.35 nm.

(2) Stanene on Ag_2Sn surface alloy by deposition [2]: The lattice parameters of Ag_2Sn surface alloy and free-standing stanene are close to each other. The Ag(111) easily react with Sn atoms on annealing, while the Ag_2Sn surface alloy is chemically inert against the Sn atoms. Thus, the Ag_2Sn surface alloy is physically and chemically ideal surface for epitaxial growth of stanene. We have successfully prepared large area planar stanene on Ag_2Sn surface alloy by Sn deposition.

(3) Plumbene on $Pd_{1-x}Pb_x$(111) alloy surface by deposition and segregation [3]: The bulk Pb-Pd system exists in fcc solid solution with a Pb concentration up to 10 %. The Pb atoms deposited dissolve into the Pd crystal and segregate on the surface on annealing. Through this process, plumbene is epitaxially grown on $Pd_{1-x}Pb_x$ (111) surface. The surface also exhibits a unique morphology in the STM images resembling the famous Weaire-Phelan bubble structure of the Olympic "WaterCube" in Beijing.

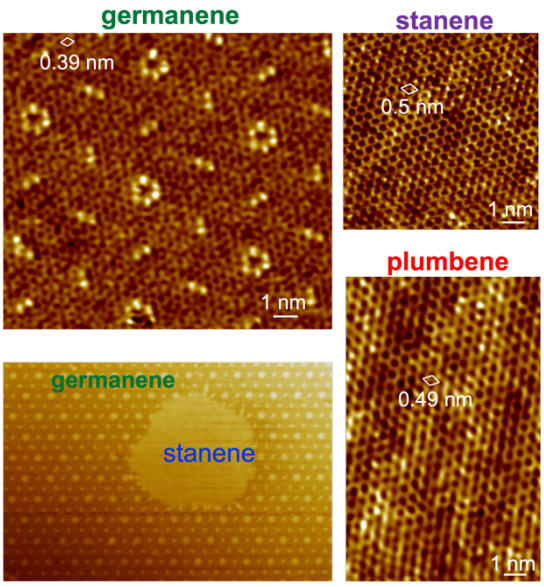

Figure 1 STM images of germanene, stanene, and their lateral heterostructure on Ag(111) and plumbene on $Pd_{1-x}Pb_x$ (111)

References:

[1] J. Yuhara et al, ACS Nano 12, 11632 (2018).
[2] J. Yuhara et al, 2D Materials 5, 025002 (2018).
[3] J. Yuhara et al, Adv. Mater. 31, 1901017 (2019).
[4] J. Yuhara and G. Le Lay, Jpn. J. Appl. Phys. 59, SN0801 (2020).
[5] T. Ogikubo et al, Adv. Mater. Inter. 7, 1902132 (2020).
[6] W. Pang et al, Appl. Surf. Sci. 517, 146224 (2020).
[7] J. Yuhara et al, Appl. Surf. Sci. 550, 149236 (2021).
[8] J. Yuhara et al, Phys. Rev. Mater. 5, 053403 (2021).
[9] J. Yuhara et al, 2D Mater. 8, 045039 (2021).
[10] S. Mizuno et al, Appl. Phys. Express 14, 125501 (2021).
[11] J. Yuhara et al, Surf. Sci., 738, 122382 (2023).

Molecular Beam Epitaxy of 2D Materials for Deep-UV Optoelectronics

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Wide bandgap semiconductors have become increasingly important due to their optical properties in the deep-UV range (UV-C, 200-280 nm), which is relevant for solar-blind optical communications and biohazard treatment. 2D materials provide opportunities to integrate UV-C optoelectronics on diverse platforms, however producing high-quality layers is still challenging. Here, we demonstrate epitaxial growth of hexagonal boron nitride (hBN)[1] and gallium selenide (GaSe)[2] by molecular beam epitaxy (MBE) as a route to scalable integration of wide bandgap semiconductors for deep-UV optoelectronics.

Step flow growth of hBN on highly oriented pyrolytic graphite (HOPG) by high-temperature MBE can produce monolayers and multilayers with micron-sized single-crystal domains. The hBN layers have high optical quality and exhibit deep-UV luminescence at 205 nm.[3] Additionally, hBN can be intentionally carbon-doped to induce single photon emission,[4] and by low-temperature scanning tunnelling microscopy (LT-STM) we observe atomically precise few-atom carbon substitutions, shedding light on the atomic structure of single photon emitters in hBN (Figure 1a). We also demonstrate growth of a new GaSe polymorph (γ'-GaSe) by MBE on epitaxial graphene/SiC and 2-inch sapphire wafers. Through *in situ* STM and angle-resolved photoemission spectroscopy (ARPES), we observe the layer-dependent valence band dispersion of 1-6L γ'-GaSe grown on epitaxial graphene, including an indirect-direct bandgap transition (Figure 1c-e). The γ'-GaSe layers exhibit resonant UV-C absorption (λ = 260 nm) which we exploit for highly sensitive photodetection.[2]

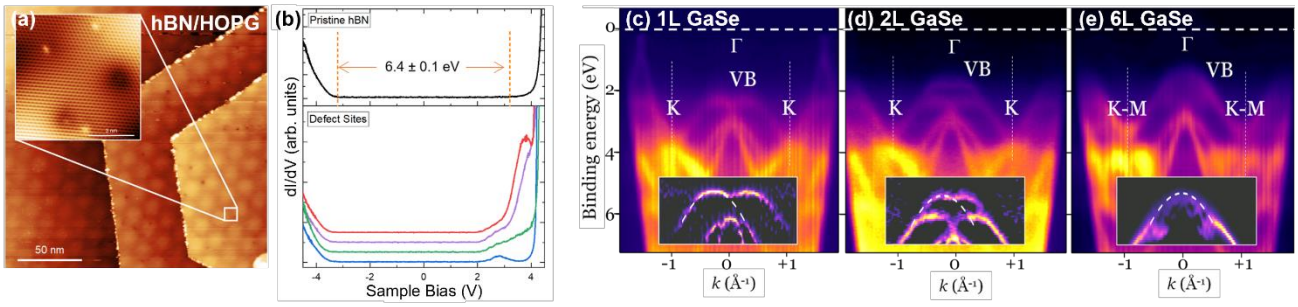

Figure 1: (a) LT-STM image of atomic scale defects in 3L hBN grown on HOPG; (b) STS point spectra showing the presence of mid-gap electronics states. (c)-(e) ARPES spectra of 1L, 2L and 6L GaSe, respectively. Insets: 2D curvature images of the upper valence band.

References:

[1] J. Wrigley, et. al., *2D Mater.* **2021**, *8*, 034001.

[2] M. Shiffa, et. al., *Small* **2023**, 2305865.

[3] A. Rousseau, et. al., *2D Mater.* **2024**, *11*, 025026.

[4] N. Mendelson, et. al., *Nat. Mater.* **2021**, *20*, 321.

2d silicon, germanium, and pnictognes by chemical methods

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The Xenes are rapidly developing family of monoelemental 2D materials. The chemistry of graphene as well as other monoelemental materials from group of tetrels and pnictogens will be shown in detail describing various strategies for its synthesis and chemical exfoliation. The differences between the exfoliation of pnictogens and tetrels will be described using chemical and mechanical exfoliation methods. In addition, the methods for the synthesis of all main group of 2D compounds and techniques of crystal growth will be presented.

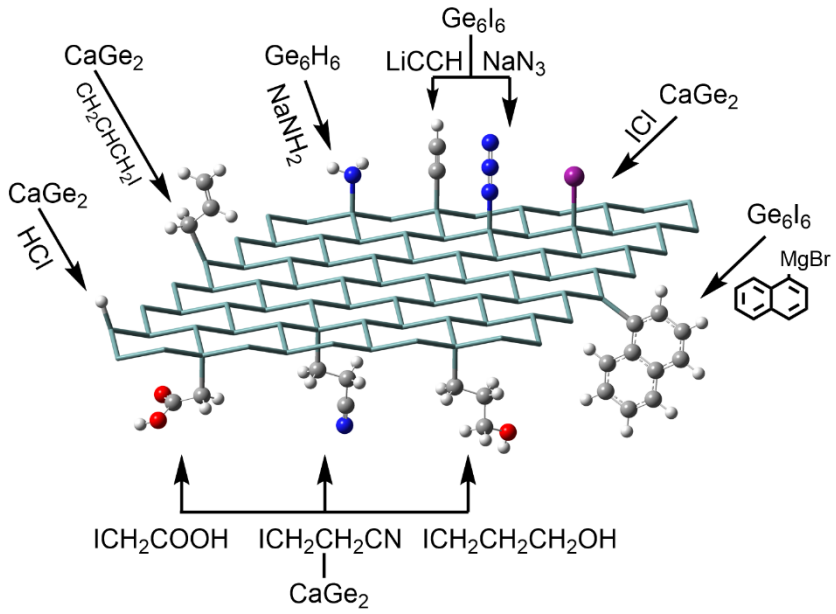

Figure 1. The possible functionalization methods for 2D silicon and germanium.

Strategies for tuning the CVD synthesis of 2D transition metal dichalcogenides in a hot-wall tube reactor

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In the family of 2D materials, transition metal dichalcogenides (TMDs), consisting of one transition metal atom bonded with two chalcogen atoms in their basic unit, play a pivotal role for next generation technology devices in many fields, since the fine control of their structure, composition, and dimensionality directly reflects on, sometimes unique, changes in their functional properties, such as the electrical, optical, optoelectronic [1] or thermoelectric response [2]. For instance, a 2D TMD specific phase structure dictates its insulating, semiconducting or (semi)metallic character; or the number of atomic layers drives the indirect-to-direct bandgap transition at the monolayer limit.

However, to transfer such remarkable results to the market, the development of affordable processes where the controlled synthesis of high-quality TMDs is achieved over large areas is mandatory. Recent research reports that, among the different routes, methods based on chemical vapor deposition (CVD) have the potential to attain this scope [3].

Here, we show our capability to obtain the synthesis of TMDs with controlled and selected properties by using CVD in hot-wall tube furnaces within optimized recipes, towards the establishment of standard protocols. We focus on MoS_2, and XTe_2 (X=Mo, Pt, Ni) as exemplar TMDs, because of their relevance, interest, and maturity for perspective applications. We introduce and discuss the role of reagents as solid powders or in solutions, the introduction of organic and inorganic promoters to facilitate the 2D growth of TMDs, the geometry in the reaction tube, and the process parameters (carrier gas flux, temperature, pressure, …). While the use of chalcogen and metal reagents as powder leads to the synthesis of isolated domains as large as hundreds of μm size [4] on flat or patterned substrates [5], with coverage up to cm^2 areas with an optimized process, the chalcogenization of pre-deposited metal thin films grants the synthesis of 2D TMDs over areas as large as the sample substrate with a highly uniform thickness. The role of chalcogen partial pressure and geometrical constrain impacts on the selectivity of the process for the synthesis of single phase TMD, such as for $MoTe_2$ 1T or 2H phase [6]. Finally, optimized temperature windows are fundamental for the high-quality synthesis of 2D TMD layers and 2D TMD heterostructures.

References:

[1] M. Zhao, Advances in Two-Dimensional Materials for Optoelectronics Applications, Crystals 12, 1087, 2022, doi:10.3390/cryst12081087
[2] W. Zhou, Recent Progress of Two-Dimensional Transition Metal Dichalcogenides for Thermoelectric Applications, 10, 842789 (2022) doi: 10.3389/fphy.2022.842789
[3] You et al., Synthesis of 2D transition metal dichalcogenides by chemical vapor deposition with controlled layer number and morphology, *Nano Convergence* 5, 26, 2018, doi:10.1186/s40580-018-0158-x
[4] P.P. Tummala et al., Application-Oriented Growth of a Molybdenum Disulfide (MoS_2) Single Layer by Means of Parametrically Optimized Chemical Vapor Deposition, *Materials* 13, 2786, 2020, doi:10.3390/ma13122786
[5] P.P. Tummala et al., Ambient Pressure Chemical Vapor Deposition of Flat and Vertically Aligned MoS_2 Nanosheets, *Nanomaterials* 12, 973, 2022, doi:10.3390/nano12060973.
[6] P.P. Tummala et al., Large Area Growth and Phase Selectivity of $MoTe_2$ Nanosheets through Simulation-Guided CVD Tellurization, A*dv. Mater. Interfaces* 10, 2200971, 2023, doi: 10.1002/admi.202200971.

Mixed-Dimensional Heterostructures for Electronic and Energy Technologies

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Layered two-dimensional (2D) materials interact primarily via van der Waals bonding, which has created new opportunities for heterostructures that are not constrained by epitaxial lattice matching requirements [1]. However, since any passivated, dangling bond-free surface interacts with another via non-covalent forces, van der Waals heterostructures are not limited to 2D materials alone. In particular, 2D materials can be integrated with a diverse range of other materials, including those of different dimensionality, to form mixed-dimensional van der Waals heterostructures [2]. Furthermore, chemical functionalization provides additional opportunities for tailoring the properties of 2D materials and the degree of coupling across heterointerfaces [3]. In this manner, a variety of optoelectronic and energy applications can be enhanced including photodetectors, optical emitters, supercapacitors, and batteries [4-7]. Furthermore, mixed-dimensional heterostructures enable unprecedented electronic device function to be realized including neuromorphic memtransistors, mixed-kernel heterojunction transistors, and moiré synaptic transistors [8-10]. In addition to technological implications for electronic and energy technologies, this talk will explore several fundamental issues including band alignment, doping, trap states, and charge/energy transfer across mixed-dimensional heterointerfaces.

References:

[1] D. Lam, e*t al.*, *ACS Nano*, **16**, 7144 (2022).
[2] M. I. B. Utama, *et al.*, *MRS Bulletin*, **48**, 905 (2023).
[3] M. I. B. Utama, *et al.*, *Nature Communications*, **14**, 2193 (2023).
[4] K.-Y. Park, *et al.*, *Advanced Materials*, **34**, 2106402 (2022).
[5] L. Kuo, *et al.*, *Advanced Materials*, **34**, 2203772 (2022).
[6] S. V. Rangnekar, *et al.*, *ACS Nano*, **17**, 17516 (2023).
[7] L. E. Chaney, *et al.*, *Advanced Materials*, **36**, 2305161 (2024).
[8] X. Yan, *et al.*, *Advanced Materials*, **34**, 2108025 (2022).
[9] X. Yan, *et al.*, *Nature Electronics*, **6**, 862 (2023).
[10] X. Yan, *et al.*, *Nature*, **624**, 551 (2023).

MXenes and other two-dimensional materials in Halide Perovskite Photovoltaics

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Due to their excellent optical and transport properties, as well as their easy tunability of electronic properties and defect tolerance, halide perovskites have rapidly become a reference material for third-generation photovoltaics. Perovskite solar cells (PSCs) are realized by depositing a series of different layers, including the perovskite absorber, hole and electron transporting materials, and electrodes. Interfaces play a crucial role in the performance of this multi-layered structure. Therefore, controlling the interface properties is of fundamental importance. In this presentation, I will discuss recent advances in the use of graphene and other 2D materials, such as MoS_2 and MXenes, to control interface properties and improve the performance and stability of PSCs. Through multiscale experimental investigations, we have found that GRMs can be used to tune interface properties, reduce ion migration, and modify the work function of the perovskite absorber and charge transporting layers. These aspects directly impact the final efficiency and stability under accelerated stress tests. The use of 2D materials can also be extended to large area modules, as well as perovskite/silicon tandem cells. This approach has been successfully employed in a solar farm with 0.5 sqm panels that was monitored for almost one year in Crete.

References

[1] Agresti, A. et al. Two-dimensional (2D) material interface engineering for efficient perovskite large-area modules. ACS Energy Lett. 4, 1862–1871 (2019).
[2] Najafi, L. et al. MoS_2 quantum dot/graphene hybrids for advanced interface engineering of a $CHNH_3PbI_3$ perovskite solar cell with an efficiency of over 20%. ACS Nano 12, 10736–10754 (2018).
[3] Agresti, A., Pazniak, A., Pescetelli, S. et al. Titanium-carbide MXenes for work function and interface engineering in perovskite solar cells. Nature Mater. 18, 1228–1234 (2019).
[4] D. Saranin et al. “Transition metal carbides (MXenes) for efficient NiO-based in-verted perovskite solar cells” Nano Energy 82, 105771 (2021)
[5] S. Pescetelli et al. Synergic use of two-dimensional materials to tailor interfaces in large area perovskite modules, Nano Energy 95, 107019 (2022)
[6] A. Yukasheva, D. Saranin et al. Photo Stabilization of p-i-n Perovskite Solar Cells with Bathocuproine: MXene Small 18, 2201730 (2022)
[7] S. Pescetelli, A. Agresti, G. Viskadouros. et al. Integration of two-dimensional materials-based perovskite solar panels into a stand-alone solar farm. Nauret Energy 7, 597–607 (2022).

Ultrafast Photophysics of Two-dimensional Semiconductors

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Atomically thin transition-metal dichalcogenides (TMDs) exhibit strong light–matter interaction and pronounced excitonic behavior. Their functional properties depend crucially on their response to external stimuli that drive them out of equilibrium. Here, I review the ultrafast photophysics of 2D semiconductors and its investigation using femtosecond optical spectroscopy. Particular emphasis will be placed on the formation and relaxation dynamics excitons, trions, and further many-body effects and their control via external parameters, as well as inter-layer charge transfer processes in heterostructures.

Point defect and proximal interface induced modification of Er^{3+} optical transitions in single crystal Er_2O_3

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Rare earth ions, such as Er^{3+}, are gaining increased attention for their potential capacity to function as qubits within solid-state devices [1]. This is due largely to the fact that the 4f-4f electronic transitions in rare-earth ions are well-shielded from their environment by filled 5s and 5p orbitals which permits the 4f-4f electronic transitions to retain atomic-like character with low spectral diffusion. Recent work characterized the basic atomic level processes involved in the temperature dependence of Er^{3+} optical transitions in Er_2O_3 single crystal thin films [2]. Here, we report the influence of defects and proximal interfaces, on the temperature dependance of photoluminescence (PL) emission intensity of Er^{3+} in the Er_2O_3 thin films, which is observed to alter the photophysical properties of Er^{3+}. Unexpectedly, the photoluminescence intensities arising from specific optical transitions were observed to be significantly enhanced as a function of defect concentration. In addition by varying the thickness of the thin film a surprising quenching was observed at decreased thicknesses. These phenomena are discussed in terms of the influence of defects on the crystal site symmetry of the host lattice and on the deviations from crystallinity near interfaces.

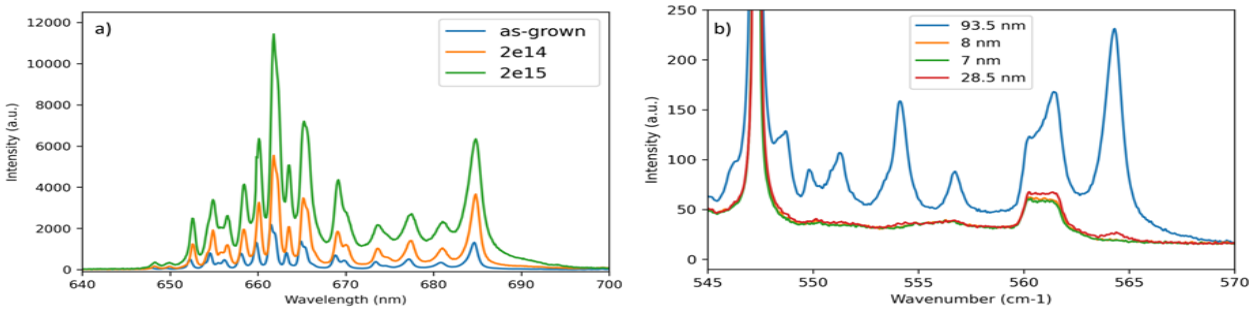

Figure 1: (a) Defect-induced enhancement of the PL from the $^4F_{9/2}$ $^4I_{15/2}$ transition manifold of Er^{3+} in Er_2O_3. The labels 2e14 and 2e15 refer to the irradiated 30 keV He^+ dose in cm^{-2}. (b) The observed quenching of photoluminescence from the $^4S_{3/2}$ $^4I_{15/2}$ transition manifold.

References:

[1] D. Grant et al., "Optical and microstructural characterization of Er3+ doped epitaxial cerium oxide on silicon" *APL Mater.* 12, 021121 (2024) doi: 1063/5.0181717

[2] A. Dodson *et al.*, "Phonon-mediated temperature dependence of Er^{3+} optical transitions in Er2O3," *Commun. Phys.*, vol. 7, no. 69, (2024), doi: 10.1038/s42005-024-01559-z.

Raman Spectroscopy at Surfaces and 2D Metallic Layers

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Raman spectroscopy is a standard analytical method to study organic and inorganic material structures. Moreover, Raman spectroscopy can be used to record phonons localized at surfaces, i.e. vibrations of the outermost few atomic planes of a material [1]. This is strongly favoured by surface specific Raman scattering mechanisms involving the surface electronic states. In collaboration with theory groups (W.G. Schmidt, Uni Paderborn, Germany and Prof. S. Sanna, Uni Giessen, Germany) ab-initio calculations of the structure and electronic bands have revealed the mechanisms of surface Raman Scattering. The comparison of experimental and computational structure, electronic properties and vibrational excitations have enabled us to conclude on surface structures, phase transitions and adsorbate induced surface modifications at 1D-metallic nanowires formed by In and Au sub-monolayer adsorbates on silicon surfaces [1-3].

More recently we have also started to investigate d-band metal surfaces (Cu(110)) and d-band 2D-metals ($Ti_2C_3T_x$-MXene). The termination of the Cu and MXene surfaces with adsorbates and their interaction with gas phase and liquid surroundings is of interest for various applications, like e.g. catalysis, sensors, energy storage. Surface termination with foreign atomic species may modify significantly Raman spectra, which in turn allows one to conclude on surface structure from spectral fingerprints [3,4]. This is shown by UHV Raman spectra for O exposure onto clean Cu(110) and for desorption of atomic terminations T_x (O, F) of the as-prepared MXene sheets by annealing. On conductive samples, Raman scattering by the charge transfer mechanism may play an important role, in addition to deformation potential scattering. This must be taken into account since Raman scattering intensities and polarization selection rules depend on the scattering mechanism.

[1] E. Speiser, N. Esser, B. Halbig, J. Geurts, W.G. Schmidt, S. Sanna, *Vibrational Raman Spectroscopy on Adsorbate Induced Low Dimensional Surface Structures*, Surface Science Reports **75** (2020) 100480.

[2] J. Plaickner, E. Speiser, C. Braun, W.G. Schmidt, N. Esser, S. Sanna, *Surface-Localized Phonon-Modes at the Si(553)-Au Nanowire System*, Phys. Rev. B **103** (2020) 115441.

[3] M. Denk, E. Speiser, J. Plaickner, S. Chandola, S. Sanna, P. Zeppenfeld, N. Esser, *Surface Resonant Raman Scattering from Cu(110)*, Phys. Rev. Lett. **128**, 21 (2022) 216101.

[4] A. Sarycheva, Y. Gogotsi, *Raman Spectroscopy Analysis of the Structure and Surface Chemistry of $Ti_3C_2T_x$ MXene,* Chem. Mater. **32** (2020) 3480.

Plasmon-enhanced Raman Spectroscopy of Low-dimensional Semiconductors

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The very small Raman scattering cross section together with the ultra-small scattering volume of nanostructures often make Raman investigations of low-dimensional structures challenging. On the other hand, plasmon-enhanced Raman techniques such as surface- and tip-enhanced Raman spectroscopy (SERS and TERS) have been continuously developed and improved since their introduction in the 1970s and in 2000, respectively. Here, the application of SERS and TERS to low-dimensional semiconductors, namely semiconductor quantum dots (QDs) and two-dimensional semiconducting transition metal dichalcogenides (TMDCs), is presented and discussed. SERS substrates consisting of ordered arrays of metallic nanostructures (MNSs) are prepared by electron beam or nanosphere lithography. Varying the geometric MNS parameters allows their localized surface plasmon resonance to be tuned and thus optimized for SERS measurements. In TERS, on the other hand, a single metallic tip of an atomic force microscope provides the highly localized plasmonic enhancement and consequently unrivalled lateral resolution on the nanoscale. In the case of QDs, the evolution from SERS measurements of QD ensembles to TERS measurements of a single QD is demonstrated. 2D TMDCs deposited on plasmonic are used, on the other hand, to illustrate the effects of strain, temperature, and hot electron doping. Combining TERS with SERS substrates allows extremely high lateral resolution to be achieved in the hot spots between the MNS and the TERS tip.

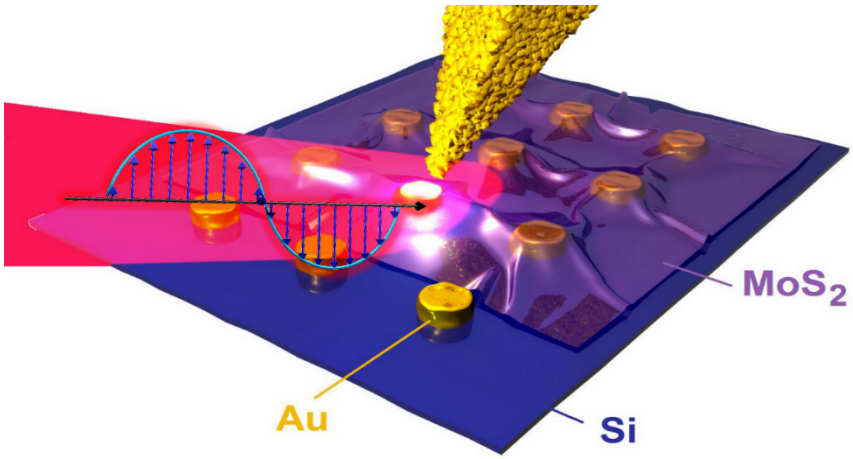

Figure 1 Sketch of a TERS experiment of a MoS_2 monolayer deposited on a plasmonic substrate.

The application of machine learning, FTIR and aperture SNOM to cancer diagnosis.

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Cancer presents a complex and significant challenge requiring a comprehensive scientific investigation. Among the various techniques available, the application of infrared (IR) aperture scanning near-field optical microscopy (aSNOM) shows potential for examining the chemical intricacies within cells with high spatial resolutions, offering valuable insights into the underlying fundamental mechanisms. Though aSNOM suffers from slow data acquisition rates, which led us to developing a methodology to first use a novel machine learning algorithm (MLA) with Fourier transform IR (FTIR) spectral images to inform our near-field experiments. This approach determines the key IR wavelengths pertinent to the problem at hand, resulting in a curated set of significant wavenumbers, which can be used in aSNOM experiments to investigate the tissues at greater spatial resolution.

While MLA techniques have had a significant impact on the study of cancer the workings of how they function are often opaque. Our MLA has been developed for the analysis of FTIR spectral images which provides some insight into the discriminating spectral characteristics of cancer cells [1]. This MLA assess the contribution of "metrics", ratios of intensities at pairs of wavenumbers, in discriminating between tissue types. When only a few metrics are required to discriminate between tissue types then these spectral intensity ratios can provide insight into the chemical differences between tissues. However, FTIR spectral images are diffraction limited and images of the same tissue were obtained at higher spatial resolution using an aperture scanning near-field optical microscope (SNOM) [2,3]. The experiments were conducted on archival formalin-fixed, paraffin embedded tissue obtained from patients with informed consent.

In one study a single metric, the ratio of the intensities of FTIR spectral images obtained at 1252 cm−1 and 1285 cm−1, was found to discriminate between oral squamous cell carcinoma nodal metastases and surrounding lymphoid tissue with sensitivities and specificities of 98.8 ± 0.1% and 99.78 ± 0.02% respectively [2]. The SNOM images confirm the importance of these two wavenumbers and reveal insight into the chemical structure of the tissue in the region of the metastatic core. In a second study [4] the MLA was able to predict which oral lesions would become malignant with an accuracy of 80%.

References:

[1] J. Ingham et. al. Infrared Physics and Technology. 102 (2019) 103007
[2] B. Ellis et. al. Analyst. 146 (2021) 4895
[3] S. Al Jedani et. al. Anal. Methods. 12 (2020) 3397
[4] B. Ellis et. al. PLoS One. 17 (2022) e02660

Xenes: from growth to applications

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Isolation of graphene paves the way to a new and unprecedentedly rich fashion of two-dimensional (2D) materials. While many of them are naturally available in the form of exfoliable single-crystal flakes, others can be artificially derived by synthetic approaches and their atomistic features tailored by design. Xenes, namely 2D single-element materials beyond graphene, are a representative case in this respect [1] but they need ad hoc processing scheme to be transferred in technological platforms. With silicene and tellurene as examples, I will describe how the Xenes can be produced by epitaxial methods. In particular, silicene stands out as a paradigmatic case for atomic structure engineering. In this respect, interface engineering through atomic Sn decoration and stannene buffering leads to the scalable epitaxy of *single-crystal silicene* and to the formation of Xene heterostructures [2]. Xene heterostructures with a top face Al_2O_3 capping layer are the enabling layout for a durable stabilization of silicene against environmental degradation via an all-around encapsulation [3]. Stabilized *silicene membranes* can be thus delaminated off from the pristine substrates and transferred to second target substrate aiming at electronic device applications. I will describe methods leading us to fabricate silicene transistors on solid-state platforms and e silicene piezoresistor on bendable substrates [4] according to the process flow in **Figure**. On the other hand, we focus on the *tellurium chemistry* to show how to grow 2D materials with unprecedented properties. Tellurium vapours transported by an inert carrier gas in a chemical vapour deposition reactor can be exploited to produce tellurium nanosheets down to the 2D level of *tellurene*. The low-temperature growth of tellurene on Au-based substrate is made to design diode cells with memristive behavior [5]. The reported cases are examples of how to engineer and configure Xene towards prototypical device targeting flexible electronics, nanophotonics, and nanoelectronics. I acknowledge funding from ERC-CoG grant n. 772261 “XFab”, ERC-PoC grant n. 101069262 “XMem”.

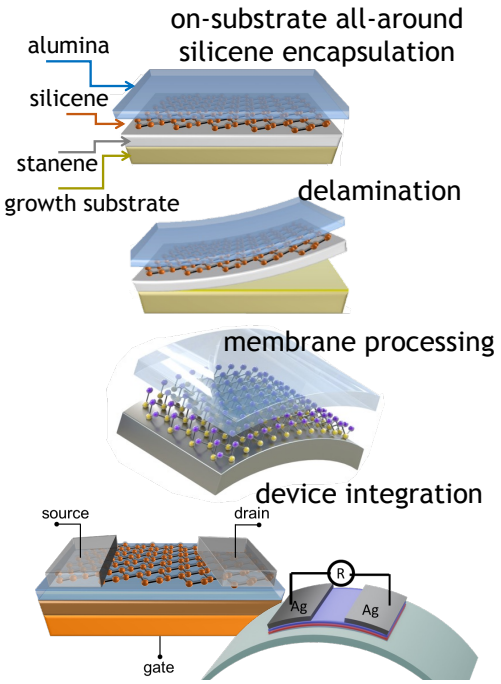

Figure Processing of a silicene nanosheet after growth, stabilization, delamination towards the extraction of durable silicene membranes that are readily transferable onto device layouts.

References:

[1] “Xenes - 2D Synthetic Materials Beyond Graphene” A. Molle and C. Grazianetti, Eds., Woodhead Publishing, Elsevier Ltd. (2022), Kidlington;
[2] S. Achilli, et al., Nanoscale (2023) 15, 11005 ; D. S. Dhungana et al., Adv. Funct. Mater. (2021) 31, 2102797;
[3] D. S. Dhunghana, C. Massetti, et al., Nanoscale Horiz. (2023) 8, 1428;
[4] C. Martella, et al., Adv. Mater. (2023) 35, 2211419 ;
[5] S. Ghomi, et al., submitted (2024).

POSTER SESSION

Synthesis of large-area MoS_2 films via CVD and L-CVD

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The realm of low-dimensional systems, particularly two-dimensional (2D) materials, has revolutionized the field of material science due to their unique and extraordinary properties, often significantly diverging from their bulk counterparts. Transition metal dichalcogenides (TMDs), exemplified by molybdenum disulfide (MoS_2), represent a fascinating class of 2D materials exhibiting exceptional electrical and optical properties that can be tailored depending on their specific composition and dimensionality. The indirect-to-direct bandgap transition in the monolayer regime, combined with their considerable carrier mobility and efficient on/off switching capabilities, positions TMDs as promising candidates for next-generation optoelectronic and photonic devices. While techniques like mechanical exfoliation have been instrumental in initial research, their scalability is limited and achieving large-area, high-quality TMD films remains a significant hurdle for practical applications. Here, we will present two different techniques aiming at the growth of large-area MoS_2 films.

Firstly, we employ conventional AP-CVD where MoO_3 and sulfur powders were used as precursors and perylene-3,4,9,10-tetracarboxylic acid tetrapotassium salt (PTAS) as seeding promotor to obtain large-area coverage of high-quality MoS_2 with orientable growth (**Figure 1a**). [1]

In a second approach, we used a solution of ammonium heptamolybdate (AHM) as the molybdenum precursor in a liquid precursor CVD process (L-CVD). The utilization of different inorganic salts as seed promoters was investigated by focusing on the thickness, morphology, uniformity and degree of coverage of the grown MoS_2. Under optimized growth parameters, we achieved high surface coverage with the lowest thickness of a two-layer (~1.4 nm) MoS_2 film (**Figure 1b**). [2]

Refining TMD synthesis methods to achieve high-quality, wafer-scale films will be essential for the practical application of these promising materials.

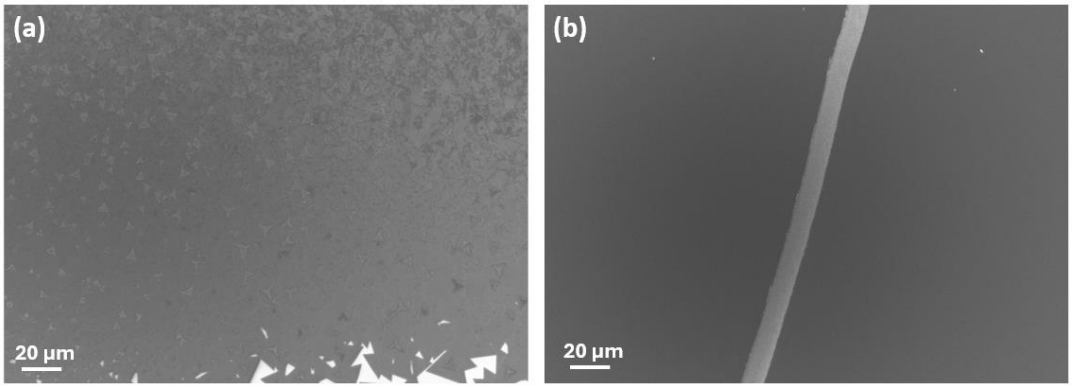

Figure 1. SEM images for CVD (a) and L-CVD (b - scratched film) grown MoS_2 layers

References:

[1] P.P. Tummala et al., "Ambient Pressure Chemical Vapor Deposition of Flat and Vertically Aligned MoS_2 Nanosheets", *Nanomaterials*, 12, 973, 2022.

[2] A. Cataldo et al., "Effects of inorganic seed promoters on MoS_2 few-layers grown via chemical vapor deposition", *Journal of Crystal Growth*, 627, 127530, 2024.

Study of the optical properties of epitaxial heterostructures based on IV-group semiconductors for photovoltaic applications

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For the last fifteen years, ternary Si-Ge-Sn alloys have been the subject of extensive research for a variety of applications, such as LEDs, photodiodes, tunnelling field-effect transistors, Si photonics (monolithically integrated on-chip laser light source [1]) and solar cells.[2]
Owning to their three elements, $Si_xGe_{1-x-y}Sn_y$ alloys offer the possibility to engineer independently the band structure and the lattice constant,[3] thus opening new possibilities for the deposition of high-quality $Si_xGe_{1-x-y}Sn_y$ layers on different substrates.
In photovoltaics, this means that Si-compatibility in direct-gap semiconductors could be achieved, thus bringing forth a new revolution in the field.
Unfortunately, serious issues in the deposition of these alloys have slowed down the research and their optical and structural properties are still unclear.
Addressing this knowledge gap, we conducted a systematical investigation of $Si_xGe_{1-x-y}Sn_y$ heterostructures with different composition through Raman and photoluminescence spectroscopies. The results revealed information on the molar fraction dependencies of energy gaps and film stress.

[1] O. Moutanabbir *et al.*, "Monolithic infrared silicon photonics: The rise of (Si)GeSn semiconductors," *Appl Phys Lett*, vol. 118, no. 11, Mar. 2021, doi: 10.1063/5.0043511.

[2] C. I. Ventura, J. D. Q. Flores, J. D. Fuhr, and R. A. Barrio, "Electronic structure of Ge1-x-ySixSny ternary alloys for multijunction solar cells," *Progress in Photovoltaics: Research and Applications*, vol. 23, no. 1, pp. 112–118, Jan. 2015, doi: 10.1002/pip.2405.

[3] S. Wirths, D. Buca, and S. Mantl, "Si-Ge-Sn alloys: From growth to applications," *Progress in Crystal Growth and Characterization of Materials*, vol. 62, no. 1. Elsevier Ltd, pp. 1–39, Mar. 01, 2016. doi: 10.1016/j.pcrysgrow.2015.11.001.

Chiral photocurrents and photogalvanic effect in bidimensional materials for photonics devices based on topological materials

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Topological effects intrigue physicists and materials scientists for their unique properties spanning from fundamental physics to novel applications. A technique to investigate chirality related phenomena, including topologically interesting effects, consists in the measurement of the current generated by the circular photo galvanic effect, where a spontaneous photocurrent is created by shining circularly polarized light on the material. After a seminal work on Bi2Se3,[1] several other scientists used this technique to investigate other materials,[2] such as elemental tellurium.[3] We developed a system for the measurement of the photogalvanic current in topological insulators and performed tests on tellurium, observing photocurrents which can be attributed to this peculiar phenomenon.

1. McIver, J.W.; Hsieh, D.; Steinberg, H.; Jarillo-Herrero, P.; Gedik, N. Control over Topological Insulator Photocurrents with Light Polarization. Nature Nanotech 2012, 7, 96–100, doi:10.1038/nnano.2011.214.

2. Aftab, S.; Hegazy, H.H.; Iqbal, M.Z. Recent Advances in 2D TMD Circular Photo-Galvanic Effects. Nanoscale 2023, 15, 3651–3665, doi:10.1039/D2NR05337C.

3. Ma, J.; Cheng, B.; Li, L.; Fan, Z.; Mu, H.; Lai, J.; Song, X.; Yang, D.; Cheng, J.; Wang, Z.; et al. Unveiling Weyl-Related Optical Responses in Semiconducting Tellurium by Mid-Infrared Circular Photogalvanic Effect. Nat Commun 2022, 13, 5425, doi:10.1038/s41467-022-33190-3.

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Moiré-induced Dirac cones replicas and minigaps opening in graphene/hBN superlattices

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Moiré superlattices, can be created by stacking two or more two-dimensional (2D) layered materials with a small twist angle and/or a slight lattice mismatch. The presence of moiré pattern results in the formation of a long range potential, which affects the dispersion of the energy levels. As a consequence of this interaction, a pletora of novel phenomena and unique functionalities [1], like strongly correlated phases [2] unconventionsl superconductivity and topological states [3], and exotic excitonic states [4] can be observed in in these systems. The aim of this study is to demonstrate that the existence of a moiré pattern in a graphene/hBN heterostructure has a substantial influence on the energy levels dispersion of the system. Evidences show that this influence goes beyond the coupling between the planes and the rehybridization of levels that can be expected in van der Waals heterostructures. Significant impact on the energy levels dispersion of graphene within an energy range inside the hBN gap, where only contributions from C atoms are expected to be present, is observed. By means of DFT calculation this study demonstrates that the moiré potential results in the formation of six replicas [5] of the graphene Dirac cones around the K-K' point of the 1BZ of graphene, which are separated by a reciprocal space superlattice vector $\mathbf{G_m}$ from the main cone. The intersection between the main cone and its replicas result in the opening of minigaps in the energy levels of graphene, without the direct interplay of the interaction with the hBN states. The relative positions of these minigaps is dependent on the moiré reconstruction of the system and can be tailored by tuning the rotation angle between the layers.

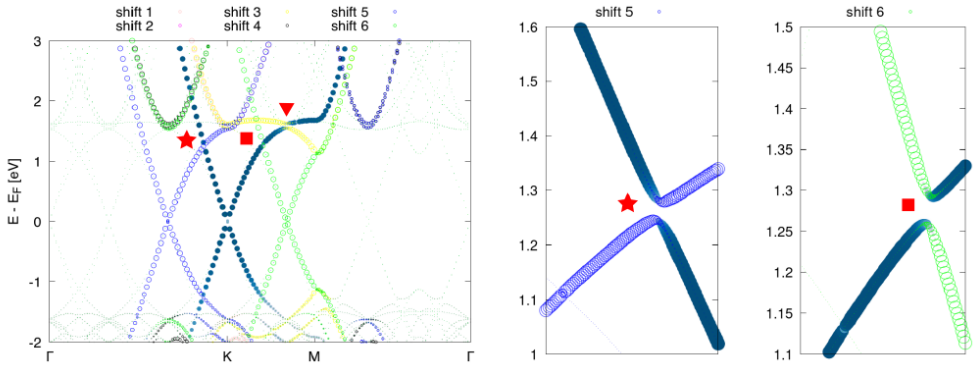

Figure 1 Minigap openings at the intersection between Dirac cone and its replicas

References:

[1] Lifu Zhang, Ruihao Ni, and You Zhou, Journal of Applied Physics 133.8 (2023)
[2] Yuan Cao et al., Nature 556.7699 (2018), pp. 80–84
[3] Yuan Cao et al., Nature 556.7699 (2018), pp. 43–50
[4] Yuan Cao et al., Science advances 3.11 (2017), e1701696
[5] Ivo Pletikosić et al., Physical review letters 102.5 (2009), p. 056808

Unveiling the optical secrets of ice sufaces: insights from advanced computational approaches

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Despite its ubiquitous presence, fundamental questions persist regarding the structure and properties of ice. Several research groups have investigated the proton order and proton disorder of different ice surfaces to better understand the behavior of ice at low temperatures [1-4]. Understanding how ice surfaces interact with light is pivotal for various applications, ranging from climate modeling to material science.
This study employs advanced computational methods, including Density Functional Theory (DFT) and beyond-DFT approaches such as GW and BSE, to investigate the equilibrium geometry, electronic structure, optical properties, and excitonic wave functions of ice surfaces. Additionally, Surface Anisotropic Reflectivity (RAS) is analyzed to uncover how variations in surface proton distribution affect their optical properties. Our primary objective is to elucidate the intricate relationship between surface structure and optical behavior, particularly focusing on how variations in surface proton distribution impact optical spectra. By examining different surfaces characterized by varying order parameters S_{OH}, which quantify the distribution of dangling OH bonds, we aim to understand how alterations in surface proton distribution influence optical properties. Our findings promise to deepen our understanding of ice's optical characteristics, with potential implications for diverse scientific disciplines.

Keywords: *Ice surfaces, optical properties, DFT, GW calculations, BSE, excitonic wavefunctions, RAS*

[1] Buch, V., et al. "Proton order in the ice crystal surface." Proceedings of the National Academy of Sciences 105.16 (2008): 5969-5974.
[2] Pan, Ding, et al. "Surface energy and surface proton order of ice I h." Physical review letters 101.15 (2008): 155703.
[3] Pan, Ding, et al. "Surface energy and surface proton order of the ice Ih basal and prism surfaces." Journal of Physics: Condensed Matter 22.7 (2010): 074209.
[4] Garbuio, Viviana, et al. "Proton disorder in cubic ice: Effect on the electronic and optical properties." The Journal of chemical physics 143.8 (2015).

Hydrogenated graphene superlattices: electronic and optical properties

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Contemporary mobile networks and emerging wireless technologies (internet of things etc.) require broadband channels to rapidly exchange a huge amount of data [1,2]. Harnessing frequencies from 0.1 to 10 THz has potential to increase the state-of-the-art high speeds by 2 orders of magnitude [3]. However, despite the latest advancements in THz technology [4], we still lack proper materials to realize suitable THz photonic components. The route to compact THz devices is seen in the usage of carbon nanostructures as building blocks for detectors, and emitters and passive components. Such carbon nanostructures, as nanotubes and graphene nanoribbons, exhibit unique electronic and optical properties that make them very promising candidates for THz components [5]. However, carbon nanotube and nanoribbon monolithic on-chip integration is challenging because it may result in significant change of their intrinsic properties after an embedment into a substrate. We investigate with first principles methods the successful integration of nanoribbons into a single-layer graphene and show that their electronic properties persist in the integrated structures forming a 2D graphene superlattice (Figure 1, left panel). Finally, we consider optical properties of the superlattices and their reinforcement with a monolayer hexagonal boron nitride (hBN) substrate (Figure 1, right panel).
This work is supported by EU HORIZON-MSCA-2021-PF-01 (project no. 101065500, TeraExc).

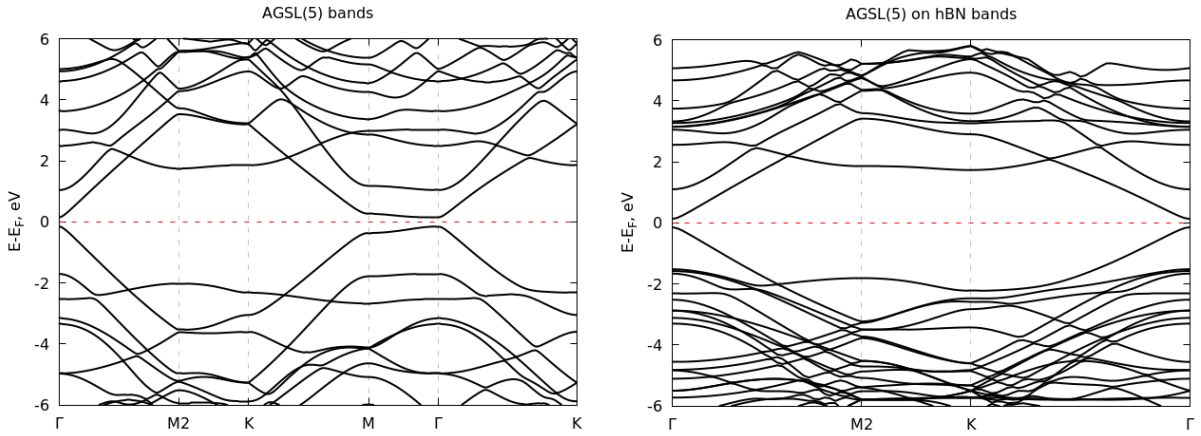

Figure 1 Electronic energy bands of hydrogenated graphene superlattice of armchair type (AGSL) with 5 C-C dimer chains in the unit cell without (left) and with (right) hBN substrate.

References:

[1] A. S. Hamza, J. S. Deogun, and D. R. Alexander, IEEE Commun. Surv. Tutorials 21, 1346 (2019).
[2] S. Ghafoor, N. Boujnah, M. H. Rehmani, and A. Davy [arXiv:1904.11441] (2019).
[3] F. Akyildiz, J. M. Jornet, and C. Han, Phys. Commun. 12, 16 (2014).
[4] S. S. Dhillon et al., J. Phys. D. Appl. Phys. 50, 043001 (2017).
[5] R. R. Hartmann, J. Kono, and M. E. Portnoi, Nanotechnology 25, 322001 (2014).

Interaction and phase transition of topological edge states in germanene nanoribbons

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Two-dimensional topological insulators conduct electricity along their edges while the bulk remains insulating [1]. This unique property offers prospects for dissipationless current transport and robust quantum computing qubits. The challenge lies in enhancing the density of these topological edge states without losing their unique properties. Utilizing germanene nanoribbon arrays [2] and scanning tunneling spectroscopy, our research probes the interaction between adjacent 1D edge states and the impact on their topological characteristics. Findings indicate that proximity leads to edge state hybridization and gap formation, shedding light on the modulation of topological protection through inter-edge interactions.

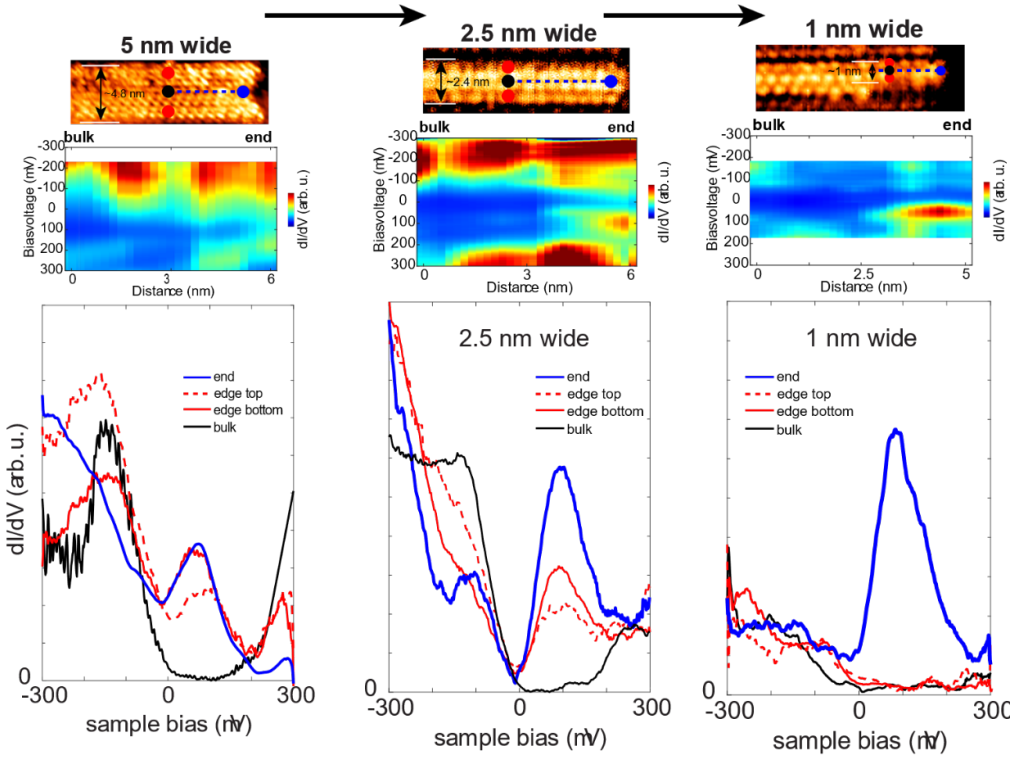

Figure. Intra-ribbon edge state interaction visualized. Transition from a wide to a small ribbon (left to right) results in the edge state disappearing, whereas the end state remains clearly visible. At small widths, this results in a 1D topological insulator with a 0D end state.

References:

[1] P. Bampoulis et al. Phys. Rev. Lett. 130, 196401 (2023)
[2] B. Poelsema et al. Phys. Rev. Materials 5, 125602 (2021)

Thiol-Based Defect Healing of WSe_2 and WS_2

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Large scale CVD grown 2D materials are now available at continuously improving quality, however native defects and natural degradation in these materials still present significant hurdles toward their implementation in electronic devices. By analyzing spectral hysteresis in gate-biased photoluminescence (PL) measurements of WSe_2, we monitored long-term trapping of charge carriers in intrinsic defect states. Measurement under variable illumination and temperature conditions, as well as using different substrates, revealed the characteristic mechanisms for trapping and release of these charges, as well as a method to estimate defect density. A thiol-based chemical process was then used to remove the native defects in CVD-grown WSe_2 and WS_2 by substituting atomic sulfur into chalcogen vacancies, which removed the observed hysteresis. The removal of defects was confirmed with X-Ray photoelectron spectroscopy measurements, among other methods, which agreed with first principles calculations. This work provides a simple and efficient method for characterizing defects and improving quality of 2D semiconductors and has the potential to impact device performance even after natural degradation.

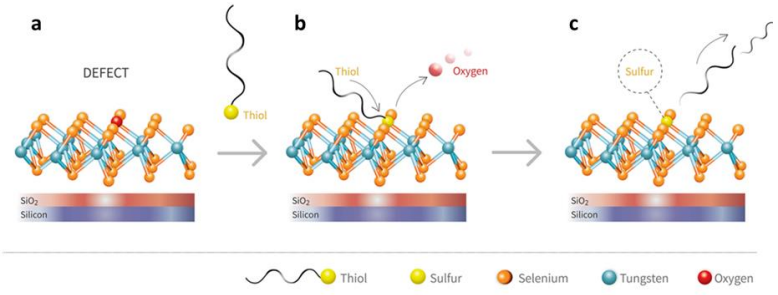

Figure 1. A schematic illustration of the WSe_2 monolayer treatments used in this work.

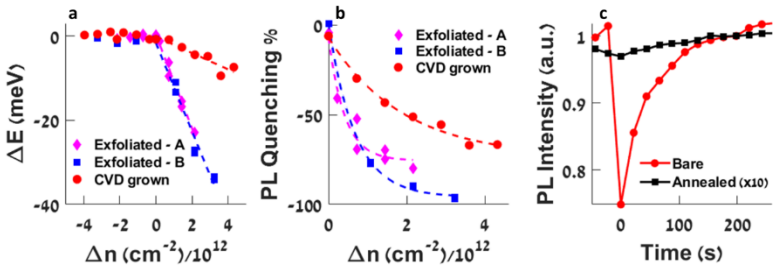

Figure 2. a-b. Spectral response to field-effect induced carrier density change. c. Effect of the defect healing process on the field-effect induced transient in PL intensity.

Maskless synthesis of van der Waals heterostructure and plasmonic arrays engineered for light harvesting on large area templates

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Large area stacking of van der Waals heterostructure arrays, based on two-dimensional (2D) Transition Metal Dichalcogenide semiconductors (TMDs), is achieved by a physical ion beam sputtering deposition process. Silica substrates, endowed with periodically faceted nano ridges, are fabricated using interference lithography and serve as templates for maskless deposition of TMD at glancing angles. This approach enables the creation of laterally confined few-layer MoS2 or WS2 nano stripe arrays. The subwavelength periodicity of the high refractive index TMD nano stripes facilitates the excitation of photonic anomalies at the onset of the evanescence condition. Consequently, light flow is effectively steered and trapped within the 2D-TMDs heterostructures and the supporting dielectric slab. Photon harvesting is engineered in the flat optics regime by optimizing the thickness of the nano stripes, which serve as optical sensitizers. In this way we achieve a resonant enhancement of optical absorption, up to a remarkable factor of 450%, when compared to a reference flat MoS2/WS2 heterostructure of equivalent thickness [1]. A similar nanofabrication approach based on interference lithography in back-etch configuration can be followed for the fabrication of plasmonic nano stripe arrays also aiming light harvesting for photocatalytic and sensing applications (Raman SERS) [2]. This result highlights the promising potential of the novel 2D-TMD and plasmonic platforms for scalable real-world applications of van der Waals heterostructures and plasmonic arrays, targeting photoconversion, photocatalysis and energy storage.

References

[1] M. Gardella et al., “Maskless synthesis of van der Waals heterostructure arrays engineered for light harvesting on large-area templates”, under submission.
[2] M.C. Giordano et al., “Self-Organized Plasmonic Nanowire Arrays Coated with Ultrathin TiO2 Films for Photoelectrochemical Energy Storage”, ACS Appl. Nano Mater. 2023, 6, 23, 21579–21586