Atomic structure of nanosystems from first-principles simulations and microscopy experiments

Physics Boat 2026

1st – 3rd June 2026
Helsinki, Finland – Stockholm, Sweden

Organizers

Dr. Arkady Krasheninnikov
Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf

Dr. Harriet Åhlgren
Helsinki Accelerator Laboratory, University of Helsinki

Prof. Hannu-Pekka Komsa
Advanced Electronics Centre, University of Oulu

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Programme

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Atomic programming of crystalline order into a crystal at the mesoscale

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Revealing the atomic structure of graphene defects by nc-AFM

I. Brihuega[1,2]

[1]Departamento de Física de la Materia Condensada Universidad Autónoma de Madrid
[2]Condensed Matter Physics Center (IFIMAC), 28049 Madrid, Spain

Atomic-scale defects are ubiquitous in graphene and often determine its ultimate electronic, thermal, and mechanical performance. In this talk, I will show how cantilever-based non-contact AFM (nc-AFM) operated in UHV at 5 K enables direct, atom-by-atom identification of defect structures with unprecedented real-space resolution, bridging the gap between idealized models and experimentally relevant interfaces. Using nc-AFM (without CO tip functionalization), we resolve a broad variety of defects in graphene grown on SiC(000-1), from topological point defects to extended grain boundaries. High-resolution imaging reveals that many defect cores are built from alternating pentagon/heptagon rings. For grain boundaries, we uncover an unexpected structural duality: stable, flat boundaries coexist with metastable configurations featuring irregular pentagon/heptagon motifs and out-of-plane corrugation [1]. First-principles modeling and simulated nc-AFM contrast attribute these metastable phases to uniaxial compressive strain, and we demonstrate in situ tip-induced switching that drives them toward the minimum-energy structure. Strikingly, although the geometric distortions are confined to only a few atoms, their influence extends over much larger length scales, highlighting how atomic defects can impact device-scale behavior.

[1] Haojie Guo et al., *Advanced Materials* e10899 (2025).

Atomic programming of crystalline order into a crystal at the mesoscale

J. Klein[1]

[1]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA, United States

Controlling the arrangement of individual atoms with lasers, ion traps, and scanning probe techniques has enabled quantum simulation and computing platforms that transcend naturally occurring configurations of matter. Yet achieving comparable atomic control within a solid and at scale remains a foundational challenge that could revolutionize the design of artificial matter.Here, we demonstrate deterministic atomic engineering inside a scanning transmission electron microscope, enabling control over atomic motion within a three-dimensional crystal [1]. Using the layered magnetic semiconductor CrSBr, an air-stable material with strong excitonic excitations and correlated magneto-electronic physics [2-5], we observe that exposure to 200 keV broad electron beam irradiation induces Cr atom displacements that generate defect complexes [6]. These include the δ_2 Cr interstitial-vacancy complex, which calculations predict to be electronically localized impurity states and optically active [7].To realize controlled displacement of Cr atoms and deterministically create these and other defect complexes, we developed several automated beam-control approaches. First, we realized a rapid, low-dose, in situ beam-control approach to position the electron beam with sub-20-picometer accuracy onto an atom or atomic column of interest [8]. We demonstrate this technique, termed "atomic lock-on," by revealing single-atom events such as displacement, recapture, and random telegraph noise in monolayer WS_2. Second, we developed a highly dose-efficient positioning algorithm, termed "stay locked-on," that allows the electron beam to be walked between user-defined lattice sites [9]. This algorithm is essential for the creation of defects in precisely lattice-ordered arrangements. Third, we developed an approach for high-frequency directional beam motion between two or more atomic columns, termed "atom steering" [1]. This enables simultaneous control and monitoring over the direction and final position of atomic displacement, which is essential for deliberately creating user-defined defect complexes.These results establish atomic engineering within the electron microscope as a practical reality. This capability opens opportunities to design quantum defects and many-body phases with tunable charge and spin interactions and to control host lattice excitations by arranging atoms in patterns that are commensurate or incommensurate with the underlying crystal order over mesoscopic and potentially even macroscopic length scales.

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Electron microscopy and spectroscopy of individual defects in low-dimensional materials

K. Suenaga[1]

[1]The University of Osaka

Properties of low-dimensional materials are largely influenced by its structural imperfections, such as defects, impurities, edges or boundaries. Hence, analytical technique at single atom level is becoming crucial to fully understand the physical/chemical performance of nano-devices. In my presentation, single atom spectroscopy by means of electron energy-loss spectroscopy (EELS) will be shown to identify the structure and chemistry of atomic defects in low-dimensional materials at their interrupted periodicities. Large variations of the atomic coordinates for novel 1D and 2D materials with will be introduced. Especially 2D nanospace in bilayer graphene is proven to be an efficient platform to stabilize different 2D phases from bulk [1]. Some of the recent examples for in situ doping experiments of low-dimensional nanomaterials will be also presented [2].

[1] YC Lin, *Advanced Materials* 2105898 (2021).
[2] Q Lin, *ACS Nano* **19**, 4845 (2025).

Versatile correlated frozen phonons from universal MLIPs for (S)TEM simulations

T. Susi[1] K. Tabata[2] N. Shibata[2]

[1]University of Vienna, Austria
[2]University of Tokyo, Japan

Harmonic phonon modes are not only critical for understanding the thermal properties of materials, but also desirable for accurate transmission electron microscopy simulations within the widely-used frozen-phonon approach. Although uncorrelated random displacements are typically sufficient for modeling diffuse backgrounds [1], the true correlated phonons may be of relevance for techniques including quantitative electron diffraction and electron ptychography [2].Although ab initio methods are routinely applied to calculate phonon dispersions for small and often non-orthogonal unit cells, (scanning) transmission electron microscopy ((S)TEM) scattering simulations typically require atomic displacements for potentially quite large orthogonal supercells. Further, since both the technical and computational effort of accurately simulating phonons from first principles is often greater than that of scattering, this severely limits their accessibility and adoption by the electron microscopy community.This challenge can be overcome with the help of force-constant potentials [3], which allow phonon properties learned for small cells to be extrapolated to arbitrary supercells. In this way, correlated phonon displacements for a given specimen model can be easily generated – including quantum-mechanical zero-point motion that is increasingly important as cryogenic instrumentation becomes more widespread. To further enhance the universality of this approach, the required forces can be efficiently calculated using recently developed foundational machine-learning interatomic potential (MLIPs), which have very recently become sufficiently accurate to model harmonic phonons for many materials across the periodic table [4].In this contribution, we establish a fully Python-based high-performance open-source workflow for including ab initio frozen phonons in electron scattering simulations using the abTEM package [5]. As demonstrations of our versatile approach, we quantify the effect of phonon correlations for selected-area and convergent-beam electron diffraction of $SrTiO_3$, and accurately model phonon-dependent electron scattering in silicon to show how correlated thermal motion between neighboring atoms preserves coherence even at elevated temperatures. Experimentally, this enables atomic-scale double-slit interferometry with a focused electron probe transmitting through a thin silicon crystal [6].

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[5] J. Madsen and T. Susi, *Open Research Europe* **1**, 13015 (2021).
[6] K. Tabata, T. Seki, T. Susi, R. Ishikawa, N. Shibata, *in review* (2026).

Defect-Mediated Tuning of Electronic and Magnetic Properties of CrSBr

M. Ghorbani-Asl[1] D. Kruklinskii[1] A. Hashemi[2] A. Krasheninnikov[1]

[1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

[2]Department of Technical Physics, University of Eastern Finland, P.O. Box 1627, FI-70211 Kuopio, Finland

Bulk CrSBr is a van der Waals semiconducting material that has recently attracted significant attention due to its intrinsic band gap, long-range magnetic ordering, and pronounced electronic anisotropy. [1,2] In addition to these intrinsic properties, it has been experimentally demonstrated that the properties can further be tuned by ion and electron irradiation in the transmission electron microscope (TEM). [3,4] We employ first-principles calculations to investigate the energetics and properties of point and line defects (e.g., edges) in monolayer CrSBr. We analyze defect formation under electron beam in the TEM by evaluating atomic displacement thresholds and calculating displacement cross-sections as functions of electron energy within the McKinley-Feshbach formalism. Furthermore, we explore the electronic and magnetic properties of finite-width nanoribbons oriented along the a, b, and d crystallographic directions. Our results reveal that nanoribbons along a direction are more stable than those along b, while cutting along d produces the most stable ribbons in the Cr-poor limit. [5] The electronic structures of CrSBr nanoribbons strongly depend on both orientation and width, with the most stable edges exhibiting half-metallic behavior. Finally, we examine the effects of Cl substitution on the electronic and vibrational properties of $CrSBr_{1-x}Cl_x$. These findings provide fundamental insights into defect-mediated tunability in CrSBr systems and open new avenues for their application in spintronic devices.[6]

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[4] F. Long, M. Ghorbani-Asl, et al., *Nano Lett.* **23**, 8468 (2023).
[5] D. Kruklinskii, M. Ghorbani-Asl, et al., *Submitted* - (2026).
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Recent advances in the theoretical modeling of STM/STS on 2D materials by applying Chen's derivative rules in the BSKAN code

K. Palotas[1,2]

[1]Institute for Solid State Physics and Optics, HUN-REN Wigner Research Center for Physics, Budapest, Hungary
[2]HUN-REN-SZTE Reaction Kinetics and Surface Chemistry Research Group, University of Szeged, Szeged, Hungary

Scanning tunneling microscopy/spectroscopy (STM/STS) are inevitable experimental methods to study the local electronic properties of various material surfaces in high spatial and energetic resolution by employing an atomically sharp probe tip.In the first part of the talk I present a new development in the BSKAN code [1] for STM/STS calculations based on first-principles electronic structure data. Recently, we implemented the revised Chen's derivative rules for electron tunneling [2] to enable computationally efficient calculations of the differential conductance dI/dV for STS simulations [3]. By taking pristine and boron- or nitrogen-doped graphene sheets as sample surfaces, the reliability of our implementation is demonstrated by comparing its results to those obtained by the Tersoff-Hamann and Bardeen's electron tunneling models. It is highlighted that the energy-resolved direct and interference contributions to dI/dV arising from the tip's electron orbitals result in a fingerprint of the particular combined surface-tip system. The significant difference between the electron acceptor boron and donor nitrogen dopants in graphene is reflected in their dI/dV fingerprints. The presented theoretical method allows for an unprecedented physical understanding of the electron tunneling process in terms of tip-orbital-resolved energy-dependent dI/dV maps that is anticipated to be extremely useful for investigating the local electronic properties of novel material surfaces in the future.In the second part of the talk I highlight recent important findings applying the BSKAN STM/STS simulation code to a variety of surfaces of current interest: (i) atomic-scale identification of nitrogen dopants in corrugated graphene [4], (ii) electron orbital insights to the effect of CO-functionalized tips in STM [5], (iii) demonstrated element-specific STM imaging of ultrathin copper oxide films [6], (iv) higher-indexed Moire patterns of electronic origin in MoTe2/graphene heterostructures [7], and (v) the STM signatures of stacked charge-density waves in 2H-NbSe2 bilayers [8].

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[7] T. T. Pham et al., *npj 2D Mater. Appl.* **6**, 48 (2022).
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Autonomous manipulation and reactions in Scanning Probe Microscopy

N. Wu[1] R. Drost[1] P. Liljeroth[1] A. S. Foster[1,2]
[1]Aalto University
[2]Nano Life Science Institute (WPI-NanoLSI)

Scanning Probe Microscopy (SPM) has been the engine of characterization in nanoscale systems in general, and the evolution of functionalized tips as a reliable tool for high-resolution imaging without material restrictions has been a breakthrough in studies of molecular systems. In parallel, machine learning (ML) methods are increasingly being applied to data challenges in SPM. In particular, the success of deep learning in image recognition tasks has led to their application to the analysis of SPM images, especially in the context of surface feature characterisation and techniques for autonomously-driven SPM. In this work, we explore the general potential of ML approaches to be used actively during SPM experiments for analysis, both in terms of feature recognition and chemical and electronic characterisation [1]. We extend this to demonstrate the autonomous construction of nanostructures through atomic and molecular manipulation, and also explore automated construction of more complex molecular systems atom-by-atom and bond-by-bond [2,3].

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[2] I-Ju Chen, Markus Aapro, Abraham Kipnis, Alexander Ilin, Peter Liljeroth and Adam S. Foster, *Nat. Commun.* **13**, 7499 (2022).
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Selective Defect Engineering in Two-Dimensional Materials: predictions from first-principles simulations

S. Ghaderzadeh[1] J. Kotakoski[2] A. N. Khlobystov[1] A. Krasheninnikov[3] E. Besley[1]

[1]School of Chemistry, University of Nottingham, Nottingham NG7 2RD, United Kingdom
[2]University of Vienna, Faculty of Physics, Boltzmanngasse 5, 1090 Vienna, Austria
[3]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden- Rossendorf, 01328 Dresden, Germany

We present a systematic investigation of displacement threshold energies in graphene and hexagonal boron nitride (h-BN) under low-energy ion-beam irradiation, covering 63 elemental projectiles from beryllium to mercury (excluding the lanthanides). This dataset establishes a broad foundation for controlled vacancy engineering and ion implantation in h-BN, with direct relevance to emerging quantum technologies including single-photon emitters and quantum sensors. Our ab initio molecular dynamics simulations reveal that chemical interactions between the incident ion and target atom dominate implantation and sputtering outcomes in the low-energy regime. While the classical binary collision approximation provides reasonable predictions for noble gases, it fails for elements that form strong transient bonds with the lattice. We further demonstrate a strong correlation between the displacement threshold energy and the vacancy formation energy when the ion approaches bonding distances. Building on these insights, we outline a strategy for selective sublattice displacement in binary compounds such as h-BN, and we identify which elements can be directly implanted by substituting specific lattice sites. Together, these results offer predictive guidance for atomic-scale defect engineering in two-dimensional materials.

Optical absorption in hexagonal-diamond Si and Ge nanowires: insights from STEM-EELS experiments and ab initio theory

M. Amato[1]
[1]Laboratoire de Physique des Solides, CNRS, Universite Paris-Saclay, Orsay, France

Hexagonal-diamond (2H) group IV semiconductors have emerged as promising materials for next-generation silicon-compatible optoelectronics, offering potential pathways toward efficient light emission in group IV platforms [1-3]. Despite growing interest in their electronic structure, a clear experimental understanding of their optical absorption properties remains lacking. In this work, I will present and discuss the first comprehensive investigation of the optical absorption of 2H-Si and 2H-Ge nanowires, combining high-resolution scanning transmission electron microscopy (STEM), monochromated electron energy-loss spectroscopy (EELS), and ab initio simulations [4].The nanowires were grown in situ within a transmission electron microscope as branches on GaAs stems, enabling exceptional control over structural quality. The resulting nanowires are single crystalline, strain-free, and virtually defect-free, with no detectable substrate contamination, providing a pristine platform for probing their intrinsic dielectric response.Our results reveal a strong enhancement in the visible-range absorption of 2H-Si compared to its cubic (3C) counterpart, with a well-defined absorption onset above 2.5 eV. For 2H-Ge, we observe a low-energy absorption onset near 1 eV, consistent with its reduced bandgap, though no distinct peak is detected at the direct bandgap transition, in line with predictions from first-principles calculations [5]. Additionally, a spectral feature around 2 eV in aloof-beam EELS is attributed to a thin 3C-Ge shell surrounding the nanowires [4].These findings mark a significant step toward understanding the structure-property relationships in hexagonal group IV nanostructures. They also provide critical insight into the optical behavior of 2H-Si and 2H-Ge, offering guidance for the development of hexagonal-phase-based optoelectronic and photonic devices.

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Tuesday 02.06.2026

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15:40	–	16:00	Michely Small polarons in single layer $MnBr_2$: substrate dependence and interaction with a super-moiré
16:00	–	16:20	Längle Properties of 2D Noble Gases
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19:20	–	19:40	Mayer Electron-beam-induced carbon doping of hexagonal boron nitride
19:40	–	20:00	Unterleutner Bridging Theory and Experiment: Point Defect Characterisation in Doped $SrTiO_3$
20:00	–	21:00	*Dinner*

From First Principles to Devices: Modeling Filamentary Switching in va-TMD Memristors

T. Lehenkari[1,2] S. Huang[1,2] T. Järvinen[1,2] K. Kordas[1] H. Komsa[1]
[1]Microelectronics Research Unit, University of Oulu, Finland
[2]Infotech Oulu, University of Oulu, Finland

Memristors are a new class of components that mimic the operation of nerve cells. They can be used to form neural networks that imitate the structure of the brain, enabling operations that are up to a hundred times more energy-efficient than current ones by circumventing the von Neumann architecture of traditional computers. This offers enormous potential for machine learning applications, enabling faster, smaller, and more environmentally friendly devices. This is especially relevant today, as already $\sim 20\%$ of the electricity consumed by data centers is taken by AI. Its ongoing rapid adoption and massive investments are expected to substantially increase global energy consumption in a world where still $\sim 80\%$ of energy is produced by burning fossil fuels. A commercially viable memristor has yet to be realized, and the search is therefore ongoing across different device types and operating mechanisms. Our research group investigates electrochemical metallization cell (ECM) type memristors based on filamentary resistance switching, with vertically grown transition metal dichalcogenides (va-TMDs) acting as the ion-conduction layer. The working principle is to form a metallic filament during device operation inside the ion-conducting layer, which significantly lowers the device resistance (by multiple orders of magnitude).Our research group not only fabricates these devices but also employs theoretical investigations to unveil the atomic-level operating mechanisms. The guiding principle in our theoretical inquiry is to begin from first principles at the atomic scale, distilling the most important physical properties and scaling them up in time and space.Using DFT, we have studied metallic defects in va-MoS_2 and translated their properties into macroscopically observable quantities such as diffusion constants and drift velocities [1]. This has yielded important insights to explain the experimental observations of volatile/non-volatile switching using different top metal electrodes in MoS_2 devices [2].A screening study of all vertically growable TMDs (MoS_2, $MoSe_2$, $MoTe_2$, WS_2, WSe_2) and top electrodes (Ag, Cu) highlighted WS_2 with a Cu top electrode as an exceptionally promising ECM memristor candidate. This observation later led to the fabrication of the first va-WS_2 ECM device in the world. Experimental research on this new device is ongoing, and the results are promising. The theoretical part has yielded a research paper that is currently under review [3].Finally, further theoretical investigation of our most studied va-TMD memristor system, MoS_2 with a Cu

top electrode, is underway. Fine-tuned machine-learning force fields (MLFFs) were used to search for and identify the most favorable Cu clustering structures in MoS_2 by enumerating and relaxing >13,000 cells. This led to the generation of a "dimer expansion" term to model Cu–Cu interactions. DFT was then used to verify these results and confirm the metallic nature of the Cu clusters. This information is now used to model the entirety of Cu filament formation in MoS_2 at device level of tens of nanometers, which could be considered the "holy grail" of the experimental side of the research project.

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Small polarons in single layer $MnBr_2$: substrate dependence and interaction with a super-moiré

A. Safeer[1] O. Güleryüz[1] G. Miao[1] W. Jolie[1] T. Michely[1] J. Fischer[1]

[1]II. Physikalisches Institut, University of Cologne, Germany

Single-layer transition metal dihalides grown on conducting substrates were shown to host small polarons [1,2]. Here, we investigate polarons in insulating single-layer $MnBr_2$ grown by molecular beam epitaxy on three different substrates, namely graphene on Ir(110), graphene on Ir(111), and Au(111). The number densities and species of polarons observed vary strongly as a function of the substrate. For $MnBr_2$ grown on Ir(110) the largest number of polaron species is observed, namely four, of which three show clear similarities with the species observed for $CoCl_2$ on graphite [1]. Polarons in single-layer $MnBr_2$ are observed up to 300 K, indicating a remarkably high barrier to thermal hopping. They can be created, converted, and moved by the STM tip when a tunneling current flows at a proper bias voltage. The presence of an equilibrium distribution of polarons within tunneling distance to a conducting substrate implies a large magnitude of the polaron formation energy. Our findings indicate that modeling of polarons in such single-layer insulators in contact with a conducting substrate requires to take the substrate explicitly into account. For graphene on Ir(110) as a substrate, mobile polarons in $MnBr_2$ are guided through the periodic potential imposed from the super-moiré resulting through the interaction of $MnBr_2$ with graphene and Ir(110) [3]. While this discovery is of fundamental interest, it implies that, in principle, it is possible to construct devices in which a laterally patterned potential may guide the motion of polarons.

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Properties of 2D Noble Gases

M. Längle[1,2] F. Castioni[1] D. Lamprecht[2,3] P. Nandi[4] K. Mustonen[2] T. Susi[2] J. Kotakoski[2] M. Kociak[1] L. Tizei[1]

[1]University Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 510 Rue André Rivière, Paris, 91405, France
[2]University of Vienna, Faculty of Physics, Boltzmanngasse 5, Vienna, 1090, Austria
[3]Institute for Microelectronics, TU Vienna, Gusshausstrasse 27-29, Vienna, 1040, Austria
[4]Laboratory of Electron Nanoscopies (LENS), University of Barcelona, Carrer de Martí i Franquès, 1, 11, 08028 Barcelona, Spain

Using low-energy ion implantation, it is possible to create small 2D noble gas crystallites by trapping them between layers of 2D materials [1]. These encapsulated noble-gas systems represent a new model platform for two-dimensional (2D) condensed-matter physics.Noble gases are non-reactive due to their outer electron shell being filled. Their interactions are governed by the van der Waals interaction, making them easy-to-understand model systems for complex processes. One example of this is condensed noble gases on cryogenic surfaces, one of the first experimental 2D systems studied in the 1960s [2]. Studying this system directly, however, is experimentally challenging. Here, 2D materials come into play. Beyond their extraordinary intrinsic properties, they can be used as ultrathin, impermeable membranes [3] confining atoms and molecules in nanometer-scale volumes [4,5]. As such, they have also been used as imaging substrates in (Scanning) Transmission Electron Microscopy ((S)TEM) studies [6,7]. In this work, multilayers of different 2D materials were irradiated with ultra-low energy noble gas ions to implant them into the van der Waals gap between the layers. This trapping between 2D materials results in 2D crystals of dense noble gases under a pressure of up to 3 GPa exerted by the graphene.Atomic-resolution STEM combined with (monochromated) electron energy loss spectroscopy (EELS) at elevated and low temperatures is used to study this system. Noble gases should be relatively non-reactive; however, in a similar system, a Kr dimer within a 1D carbon structure, it was found that the Kr-Kr bond length indicates covalent bonding after ionization via the imaging electron beam [8], in line with a recent theoretical study on covalent bonding of ionized noble gas atoms [9].We have observed indications of non-van der Waals bonding in clusters, both using EELS and by studying the atomic arrangement, which raises the question of which mechanism governs the system. Additionally, encapsulation and temperature control allow us to investigate the melting of these clusters in 2D, where we observed a surprising process involving 1D liquid chains. The results suggest that inert atoms can be forced to

bond chemically when confined at high pressures within atomically thin cavities under electron irradiation.Noble gases encapsulated between 2D materials constitute a versatile platform for exploring different phenomena in condensed-matter physics. By combining encapsulation in van der Waals materials with atomic-resolution STEM and EELS, we create a powerful playground for future 2D condensed-matter research.

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Hamiltonian learning nanoscale quantum magnets and multiorbital excitations with setpoint-dependent scanning tunneling spectroscopy

J. Lado[1]
[1]Department of Applied Physics, Aalto University, Finland

Atomic-scale quantum many body systems provide a versatile platform to explore the emergence of quantum excitations in many-body systems. Here, we establish Hamiltonian learning strategies [1,2] to extract many-body Hamiltonians directly from scanning tunnel spectroscopy, applicable both to nanoscale quantum magnets and complex nanoscale multiorbital many-body excitations. First [1], we demonstrate this methodology experimentally with an artificial triplon quantum magnet based on cobalt phthalocyanine (CoPC) molecules on NbSe2. We show that this technique allows us to extract the Hamiltonian parameters of a quantum magnet from the differential conductance, including the substrate-induced spatial variation of the exchange couplings. Second [2], we introduce a molecular Hamiltonian learning strategy that infers the microscopic Hamiltonian parameters of a single adsorbed molecule directly from the setpoint-dependence of STM-IETS data. The method leverages the systematic evolution of spectral features as the STM tip tunes the local electrostatic environment for different tip-sample distances. We demonstrate this approach on iron phthalocyanine (FePC) on ferroelectric SnTe, training our algorithm on theory spectra from a realistic multiorbital model, including spin-orbit coupling, electrostatic interactions, local crystal field, and substrate effects. The algorithm, trained solely on theoretical many-body simulations, allows for reconstructing Hamiltonian parameters directly from experimental spectra. Our results establish setpoint-dependent spectroscopy as a flexible strategy for Hamiltonian learning in nanoscale quantum materials.[1] Rouven Koch, Robert Drost, Peter Liljeroth, and Jose L. Lado, Nano Letters, 25, 36, 13435–13440 (2025) [2] Greta Lupi, Adolfo O. Fumega, Mohammad Amini, Robert Drost, Peter Liljeroth, Jose L. Lado, arXiv:2601.19371 (2026)

Four-dimensional STEM: A new approach to probe defects in synthesized 2D materials

H. Okuno[1] D. Dosenovic[1] S. Dechamps[1] A. Filicetti[1] F. Delmonte[1]
[1]Univ. Grenoble-Alpes, CEA-IRIG

Two-dimensional (2D) materials provide a versatile platform for structural engineering, where defects, stacking order, and elemental combinations can be tailored to tune physical properties. However, achieving controlled synthesis remains a key challenge, as intrinsic atomic defects become both powerful tuning parameters and unavoidable sources of discrepancies between experimental measurements and ideal theoretical predictions. Probing these defects at the atomic scale is thus essential to understand their formation and properties, but must be complemented by large-scale analysis of their distribution to build realistic structural models, where materials are described as patchworks of atomic defects that determine their general properties. Aberration-corrected scanning transmission electron microscopy (AC-STEM) has been known as a powerful and reliable technique for imaging atomic defects in atomically thin 2D layers, with a possibility to associate chemical information using spectroscopies. Recently, four-dimensional STEM (4D-STEM) has emerged as a technique that can capture local information by recording a diffraction pattern at every scanning beam position, providing quantitative data that complements atomic-scale structural and chemical imaging and also enables large-scale structural analysis. For instance, analyzing the deviation of the transmitted beam position (Center of Mass: CoM) in 4D-datasets acquired at atomic scale gives access to the local electric field around individual defects, and to the electrostatic potential and the charge density through Poisson's equation [1,2]. On a larger scale, extracting specific diffraction signals collected over extended areas allows the localization of diverse types of defects. Advances in microscopy and computational capabilities now enable the collection and processing of large datasets, but this also makes their interpretation increasingly complex and requires careful analysis combined with simulated datasets and DFT calculations to extract reliable structural and physical insights.In this talk, the application of 4D-STEM to the study of synthesized 2D materials will be demonstrated, illustrated with several examples realized in our group. Atomic-scale CoM imaging highlights the capability of 4D-STEM for quantitatively detecting negative charge accumulation around single dopant atoms in MBE-grown WSe_2 monolayers. The charge state of dopant atoms is determined by comparison with simulated datasets including DFT calculations and residual aberrations

measured by the ptychographic reconstruction of the probe [3]. Mapping domain junctions in transition metal dichalcogenide (TMD) monolayers and multilayer films demonstrates the utility of large-scale defect analysis, providing an overview of the distribution of key atomic defects identified through atomic-resolution imaging and DFT calculations. This allows the statistical correlation of structural defects with the experimentally measured electrical properties of the films [4,5].

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[3] D. Dosenovic et al., *ACS Nano* **18**, 23354 (2024).
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[5] E. Desgué et al., *arXiv* **2503**, 20659 (2025).

Electron-beam-induced carbon doping of hexagonal boron nitride

B. M. Mayer[1,2] M. Längle[1,3] U. Javed[1,4] T. Susi[1] E. H. Åhlgren[2] J. Kotakoski[1]

[1]Physik Nanostrukturierter Materialien, University Vienna, Boltzmanngasse 5, 1090 Vienna, Austria
[2]University of Uppsala,Department of Physics and Astronomy, Uppsala, Sweden
[3]University of Paris-Saclay, Paris, France
[4]University of Vienna, Vienna Doctoral School in Physics, Boltzmanngasse 5, 1090 Vienna, Austria

Hexagonal boron nitride (hBN) is a two-dimensional material structurally similar to graphene but distinguished by its wide bandgap and alternating boron and nitrogen atoms instead of carbon. Recently, hBN has gained significant interest because some of its defects have been shown to serve as single-photon emitters at room temperature. The most promising defects for quantum emitters are single-atom vacancies and substitutional atoms, with defects containing carbon impurities showing particular promise for quantum technology applications [1].This study investigates carbon doping of hBN via electron-beam-induced deposition. The high-energy electrons used for imaging in a scanning transmission electron microscope are used to create vacancies in the hBN lattice. At the same time, methane (CH_4) is introduced into the column, where the electron beam dissociates the molecules, releasing carbon atoms that migrate into the vacancies to form carbon-based structures. Time-resolved image sequences at various pressures (6^{-9} - 1^{-7} Torr) are recorded to monitor this process. These series are used to determine pore growth rates and image carbon structures in the lattice. Electron energy-loss spectroscopy (EELS) is used to verify the elemental composition.The results show that boron and nitrogen atoms are gradually replaced by carbon. Surprisingly, increased methane concentration slows nanopore growth during the experiment and leads to a new type of defect–triangular carbon-terminated pores. Our experiments show that these pores are induced by hydrogen in the column.

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Bridging Theory and Experiment: Point Defect Characterisation in Doped $SrTiO_3$

E. Unterleutner [1] B. Haas[2] A. Gladyshev[2] M. McCauley[2] L. Wibmer[3] M. Aichhorn[3] F. Hofer[1,4] C. T. Koch[2] G. Kothleitner[1,4] D. Knez[1]

[1]Institute of Electron Microscopy and Nanoanalysis, Graz University of Technology, Graz, Austria
[2]Department of Physics and Center for the Science of Materials Berlin, Humboldt-Universitaet zu Berlin, Berlin, Germany
[3]Institute of Theoretical and Computational Physics, Graz University of Technology, Graz, Austria
[4]Graz Centre for Electron Microscopy (ZFE), Graz, Austria

Defect engineering is a pivotal strategy for tailoring the electronic and magnetic properties of complex oxides. However, bridging the gap between microscopic point defect properties and macroscopic material behavior remains a significant challenge. To establish this link, first-principles modelling via density functional theory (DFT) is essential, as it provides the necessary structural and electronic foundation to interpret advanced microscopy measurements and predict bulk functionality. While crucial for optimizing performance, the reliable characterization of individual defects in the bulk is often hindered by limitations in spatial resolution, signal sensitivity, and experimental stability, necessitating the development of new experimental strategies. Addressing these experimental requirements, we performed atomic-resolution 4D-STEM experiments on $SrTiO_3$ doped with 0.5 wt% tantalum (Ta) using a Nion HERMES microscope operating at 60 kV with a semi-convergence angle of 36 mrad. Meticulous optimization of experimental conditions and the preparation of exceptionally thin specimens, limited to only a few nanometres in thickness, were essential to ensure the detection of subtle defect signals.[1] We employ DFT calculations[2] to determine the relaxed atomic structures of relevant point defects, such as Ta substitutional dopants and associated Sr vacancies. These DFT-derived geometries serve as input for multislice simulations of electron scattering[3], enabling the prediction of defect-induced modifications to the angular scattering distribution.[4] We demonstrate that these sub-angstrom atomic displacements produce characteristic diffuse scattering contributions (Huang scattering[5]), which significantly influence the momentum-resolved signal measured in 4D-STEM.[6] By incorporating these structural distortions into the simulations, we identify defect-specific scattering signatures and design optimized virtual detectors to enhance sensitivity to individual point defects. By combining DFT-derived defect structures, multislice simulations, and 4D-STEM, we establish a robust framework for the detection and characterization of individual point defects. This integration of first-principles modelling with advanced electron microscopy

provides a pathway toward quantitative defect analysis in complex oxides and other functional materials.

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Wednesday 03.06.2026

chair: Lado

9:00 – 9:40 **Louie**
Tuning Magnetism with Patterned Defect Engineering in Graphene Nanoribbons

9:40 – 10:20 **Fischer**
Atomic-Scale Structure and Magnetic Order in Novel 2D Materials

10:20 – 10:40 Tran
Ion Beams Through Nanopore Masks: A Platform for Nanoscale Patterning and Defect Dynamics in Two-Dimensional Materials

10:40 – 11:20 *Coffee*

chair: Fernández-Rossier

11:20 – 12:00 **Meunier**
Graph Embedding Tensor: Unifying Topological Description, Symmetry Detection, and Structure Generation for Two-Dimensional Carbon Allotropes

12:00 – 12:20 Bellani
Microscopy and vibrational spectroscopy of GaN nanowires on silicon toward scalable quantum devices

12:20 – 12:40 Javed
Origin of round and triangular irradiation induced pores in hexagonal boron nitride (hBN)

12:40 – 13:00 *Closing*

13:00 – 14:00 *Lunch*

Tuning Magnetism with Patterned Defect Engineering in Graphene Nanoribbons

S. G. Louie[1,2]

[1]Department of Physics, University of California at Berkeley
[2]Materials Sciences Division, Lawrence Berkeley National Laboratory

Atomically thin quasi-one- and two-dimensional materials host a wide range of quantum phenomena. In graphene nanostructures, defects can induce emergent magnetic behavior by generating low-energy zero modes (ZMs), often of topological origin. Interactions among patterned ZMs shape frontier bands and enable magnetically ordered phases. Here, we present two recent studies that exploit patterned defect motifs to control quantum magnetism in graphene nanoribbons (GNRs). First, combining topological classification with defect engineering, we identify a new class of zigzag-edged magnetic Janus GNRs (JGNRs). These JGNRs host diverse quantum magnetic phases – ranging from antiferromagnetism to ferrimagnetism to ferromagnetism – which can be tuned by controlling their defective edge structures, decorated with benzene-like motifs. Second, we study another noncentrosymmetric GNR in which all ZMs reside on the majority sublattice; strong electron–electron correlations drive a Stoner instability, producing a ferromagnetic insulating ground state with a sizable band gap. At elevated temperatures, a chemically induced transformation triggers an insulator-to-metal transition and suppresses ferromagnetism. Both studies represent joint theory–experiment efforts, in which theoretical predictions are validated through bottom-up synthesis and scanning probe microscopy measurements.

Atomic-Scale Structure and Magnetic Order in Novel 2D Materials

J. Fischer[1]
[1]Institute of Physics II, University of Cologne, Germany

Intrinsic magnetism in atomically thin materials has expanded the scope of 2D physics, yet exfoliation remains limited to bulk-derived phases. Molecular beam epitaxy (MBE) overcomes this constraint, enabling the synthesis of structurally distinct single-layer materials [1,2]. Controlled MBE growth of chromium sulfide and iron sulfide on graphene/Ir results in two novel 2D materials, single-layer Cr_2S_3-2D, which adopts a covalent hexagonal structure with S–Cr–S–Cr–S stacking (NiAs structure) and h-Fe_2S_2, a single-layer polymorph with two buckled honeycomb-like planes (β-CuI structure). Both are novel 2D materials with structures without bulk counterpart and their novel magnetic order is characterized by spin-polarized scanning tunneling microscopy. In my talk, I will show that Cr_2S_3-2D is the first single-layer A-type antiferromagnet – out-of-plane mag-netic moments couple ferromagnetic within each Cr plane and antiferromagnetic between Cr planes. In addition, I will show that the out-of-plane Néel vector of the antiferromagnetic order can be switched like a ferromagnet, enabled by uncompensated moments due to interface-induced charge transfer and symmetry breaking. Lastly, I will show that magnetic order in h-Fe_2S_2 is non-collinear within the 2D plane, forming an antiferromagnetic 120° Néel state. Our results demonstrate that MBE enables access to novel magnetic states beyond bulk constraints, opening pathways for engineered 2D quantum materials.

[1] Knispel et al., *Small* **21**, 2408044 (2025).
[2] Safeer et al., *Adv. Funct. Mater.* **35**, e00907 (2025).

Ion Beams Through Nanopore Masks: A Platform for Nanoscale Patterning and Defect Dynamics in Two-Dimensional Materials

T. T. Tran[1] H. Bruce[1] N. H. Pham[2] P. Persson[3] R. Holenak[1] D. Primetzhofer[1]

[1]Department of Physics and Astronomy, Ångström Laboratory, Uppsala University, Box 516, Uppsala SE-751 20, Sweden
[2]Division of Solid-State Electronics, Department of Electrical Engineering, Uppsala University, Uppsala SE-751 03, Sweden
[3]Thin Film Physics Division, Department of Physics, Chemistry, and Biology (IFM), Linköping University, Linköping, Sweden

In this presentation, we demonstrate that ion irradiation through nanopore masks not only offers a route to patterning at a truly nanoscale, but also enables fundamental studies of defect dynamics in two-dimensional (2D) materials.Deterministic patterning of 2D materials at the nanoscale is essential for applications in electronics, photonic metasurfaces, and separation membranes. However, established top-down approaches face a persistent trade-off between resolution, throughput, and cleanliness: electron-beam lithography and other resist-based patterning typically introduce residues that are difficult to fully remove from atomically thin membranes, while high-resolution focused ion/electron beams deliver excellent precision but limited scalability. Motivated by these limitations, we demonstrate a resist-free, contactless approach in which energetic Ar^+ ions transmitted through a suspended Si nanopore mask transfer exactly predefined patterns into self-supporting graphene using a broad ion beam. The method enables large-area patterning with demonstrated feature sizes down to $\sim$15 nm. Simultaneously, the irradiation drives local cleaning by coupling surface diffusion and sputtering of hydrocarbon contaminants, improving membrane cleanliness in and around patterned regions in a single step. Using the same nanopore-mask platform, we also establish an experimental geometry for fundamental defect studies by spatially separating where defects are created from where they are later analyzed. This controlled confinement of irradiation allows us to probe defect propagation in graphene under ambient conditions using selected area electron diffraction (SAED), high resolution TEM (HRTEM), and electron energy loss spectroscopy (STEM-EELS). In both uniformly irradiated and nanopore-masked samples, ion damage produces a global lattice expansion, with tensile strain reaching $\sim$0.8% at intermediate defect densities before relaxing at higher damage levels. Strikingly, we observe reduced crystallinity and clear defect-density gradients in regions outside the directly irradiated areas, indicating room-temperature migration of irradiation-induced vacancies over distances of order $\sim$100 nm. These observations support

a strain-assisted vacancy migration mechanism, in which ion-induced lattice strain lowers the effective migration barrier. In addition, the data point to an active role of mobile adatoms, which can partially heal the lattice through vacancy – adatom recombination.

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Graph Embedding Tensor: Unifying Topological Description, Symmetry Detection, and Structure Generation for Two-Dimensional Carbon Allotropes

V. Meunier[1] L. Macmillan[1] E. C. Girão[2]

[1]Department of Engineering Science and Mechanics, Penn State University, University Park, PA, USA

[2]Departamento de Física, Universidade Federal do Piauí, Teresina, Piauí, Brazil

The exploration of two-dimensional carbon allotropes beyond graphene has generated significant interest in materials science, yet systematic enumeration and characterization of these structures remain challenging [1]. We introduce the embedding tensor Φ, a rank-3 integer tensor that provides a unique, coordinate-free representation of any three-connected two-dimensional carbon lattice [2]. Unlike traditional adjacency matrices, which cannot distinguish between topologically distinct structures with identical connectivity, the embedding tensor unifies vertices, edges, and polygonal faces into a single mathematical framework, enabling exact identification of structural isomorphism. The tensor formalism obeys summation rules derived from Euler characteristics and can be cast into a flag graph representation. This enables tolerance-free identification of wallpaper symmetries through purely algebraic operations, avoiding the numerical precision issues inherent in coordinate-based symmetry detection methods. Building on this framework, we developed an iterative add-dimer search algorithm that generates all structures with N_F faces from crystals with $N_F - 1$ faces. The algorithm automatically discards duplicates via tensor isomorphism checking and identifies non-primitive cells through symmetry analysis. By exploiting symmetry to restrict dimer insertion to symmetry-unique positions, we transform an otherwise exponential combinatorial search into a tractable approach, successfully enumerating structures up to $N_F = 7$, yielding 1,823 unique primitive cells without triangles and 12,450 total structures including triangular rings. Once candidate topologies are enumerated, approximate real-space coordinates and lattice vectors can be reconstructed analytically from Φ and sparse crossing matrices using a non-iterative least-squares approach. This provides initial geometries suitable for subsequent electronic structure or vibrational calculations. The method delivers an end-to-end pipeline from exhaustive symmetry-aware enumeration to metadata tagging and coordinate generation, requiring only integer arithmetic and avoiding floating-point tolerances until the final coordinate reconstruction step.This work establishes a rigorous mathematical foundation for high-throughput computational exploration of two-dimensional materials, with immediate applications to

carbon allotropes and potential extensions to other planar networks including boron nitride and boron–carbon–nitrogen compounds.

[1] A. Macmillan, E.C. Girão, V. Meunier, *Carbon* **203**, 611 (2023).
[2] L. Macmillan, E.C. Girão, V. Meunier, *Npj Computational Materials* **12**, 65 (2026).

Microscopy and vibrational spectroscopy of GaN nanowires on silicon toward scalable quantum devices

S. Restelli[1] B. Alloing[2] P. Coulon[2] V. Bellani[1]

[1]Università di Pavia, Dipartimento di Fisica "A. Volta" and INFN, via Bassi 6, 27100 Pavia, Italy
[2]Université Côte d'Azur, CNRS, CRHEA, rue Bernard Gregory, Sophia Antipolis, 06560 Valbonne, France

GaN nanowires (NWs) are a promising material platform for quantum photonics and sensing due to their wide bandgap, strong confinement effects, and potential for room-temperature operation. Integrating GaN NWs on silicon substrates is particularly attractive for scalable quantum technologies. Thanks to the strain relaxation at the lateral facets, NWs represent a promising solution for reducing the effect of lattice mismatch and defect formation at the nanoscale.In this work, we present a detailed structural and vibrational characterization of selectively grown GaN nanowire arrays on AlN-buffered silicon. Using a correlative approach based on scanning electron microscopy (SEM), atomic force microscopy (AFM), and micro-Raman spectroscopy, we investigate how growth conditions and substrate engineering influence nanowire morphology, base structure, and vibrational response. This provides insight into strain accommodation and defect formation mechanisms relevant for quantum device performance. Micro-Raman mapping performed on both standing and detached nanowires reveals confined phonon modes, acoustic overtones, and surface optical phonons characteristic of GaN nanostructures. These vibrational features are sensitive to nanoscale geometry, surface effects, and local strain, and provide an effective probe of nanowire structural quality.Overall, this study demonstrates how the combined use of high-resolution microscopy and vibrational spectroscopy can elucidate structure vs property relationships in GaN nanowires on silicon. The results provide experimentally grounded guidance for optimizing nanowire growth and integration, supporting the development of scalable, room-temperature quantum photonic and sensing architectures.

Origin of round and triangular irradiation induced pores in hexagonal boron nitride (hBN)

U. Javed[1,2] M. Laengle[1] V. Zobac[1] A. Markevich[1] B. M. Mayer[1,3] C. Kofler[1,2] M. Paul[1] D. Lorber[1] N. Ravindran[1,2] C. Mangler[1] T. Susi[1] J. Kotakoski[1]

[1]University of Vienna, Faculty of Physics, Vienna, Austria
[2]University of Vienna, Vienna Doctoral School in Physics, Vienna, Austria
[3]Uppsala University, Faculty of Physics, Box 516, SE-751 20, Sweden

For nearly two decades, it has been known that electron irradiation of hexagonal boron nitride (hBN) leads to the formation of triangular pores with nitrogen-terminated edges. The broadly accepted explanation was that boron is easier to displace than nitrogen, owing to their differing displacement cross-sections resulting from their mass difference and displacement threshold energies. It had also been speculated that the residual vacuum in the microscope column could play a role in the preferred removal of boron atoms, but this hypothesis was not tested until now.In this study [1], we used Nion UltraSTEM 100 in Vienna, which operates at the base pressure of 1e-10 mbar (which is three orders of magnitude lower than typical microscopes). Due to customization, it is also possible to introduce a controlled gas atmosphere of up to 1e-6 mbar around the sample without affecting the imaging conditions. We studied the electron-beam-induced pore growth in hBN at oxygen partial pressures from 1e-10 mbar to 3e-8 mbar with electron energies of 60 keV and 80 keV. In contrast to previous high-vacuum experiments, we show that electron irradiation in ultra-high vacuum (1e-10 mbar) leads to circular pores with no preference to either boron or nitrogen-terminated edges, whereas even small amounts of oxygen in the atmosphere during the experiment changes the pore shapes into triangles with nitrogen-terminated edges. These results hold for both 60 and 80 keV electron energies, and different sample types. Although pore growth at 60 keV is generally slower than at 80 keV, at the highest pressure, the growth rate appears independent of the electron energy. This indicates that at higher pressures, the pore growth is dominated by a beam-assisted chemical process rather than direct electron-beam damage.We turn to ab initio simulations to elucidate the underlying reasons for this observation. These show that oxygen atoms, created from O_2 by the electron beam, attach preferentially to B at pore edges. From this configuration, it is easier to remove the O and B together rather than just O with the electron beam, whereas the opposite is true for N atoms at the edge. This explains the prevalence of nitrogen edges at higher oxygen pressures, and therefore also the observed triangular pores.Our observations show that damage in hBN under electron irradiation is a combination of physical damage caused

by electrons in the form of knock-on damage or radiolysis, and chemical etching caused by oxygen radicals, which affect boron significantly more than nitrogen. This opens the possibility of defect-engineering materials with desirable edges or atomic-scale defects by controlling both physical and chemical effects during particle irradiation.

[1] U. Javed et al., *arXiv* **2507**, 13180 (2025).

Posters

Shrirang Chokappa
: Selective defect creation in 2D hexagonal boron nitride via ultra-low energy Ar ion irradiation

Ahmad Echresh
: High-Performance Mixed-Dimensional Reconfigurable Field-Effect Transistors with Enhanced Polarity Control

Albert Elias Tronholm Edvardsen
: Quantifying the detectability of surface defects in $CuInS_2$ quantum dots through DFT-informed electron microscopy simulations

Joaquín Fernández Rossier
: Determining Energy Dispersion of Spin Excitations with Scanning Tunneling Spectroscopy

Paulina Indyka
: Linking Alkali Distribution and Mn Redox Gradients in Manganese Oxide Nanocrystals: A Combined STEM-EELS and First-Principles Study

Farzin Irandoost
: Tip recognition in NC-AFM images in liquid

Philipp Irschik
: Atomically clean free-standing two-dimensional materials through heating in ultra-high vacuum

Patrick James
: The effects of noble gas intercalation on bilayer MoS_2 sheets: A DFT study

Daniel Jansen
: Atomic-Scale Assembly of Quantum Defects in Two-Dimensional Semiconductors with the Scanning Tunneling Microscope

Clara Kofler
: From four t(w)o three: An exploration of interferometric 4D-STEM for measuring 3D variations in twisted bilayer graphene

Ondrej Krejci
: Advancing scanning probe microscopy simulations: A decade of development in probe-particle models

Daniil Kruklinskii
: Structure and Properties of Mirror-Twin Boundary Networks in Substoichiometric $MoTe_2$: Insights from First-Principles Calculations

Maxime Le Ster
: Moiré Plane Wave Expansion Model

Greta Lupi
: Molecular Hamiltonian learning from setpoint-dependent scanning tunneling spectroscopy

Rabia Nawaz
: Ultra-low energy ion irradiation of few-layer MoS2: defect production and intercalation

Pablo Planelles Prensa
: Tip-enhanced Raman Spectroscopy simulation methods

Animesh Puzari
: Orbital Ordering in 2D Multiferroic VCl3/HOPG

Nils Henrik Samuli Stenbrink
: Ferroelectric relaxation dynamics of twisted bilayer hexagonal boron nitride

Peter Sutter
: Multilayer Van der Waals Heterostructures: Opportunities Beyond the 2D Limit

Eli Sutter
: Macroscopic Tin Monochalcogenide Van der Waals Ferroelectrics: Growth, Alloys, Doping, Domain Structures, and Curie Temperatures

Tfyeche Y Tounsi

Tuning the Kondo temperature of MoS_2 mirror twin boundaries on graphene

Kuber Vyas

Spin Screening in MoS_2 Mirror Twin Boundaries on graphene on Ir(110)

Yucheng Zhang

Microscopic Image Deblurring by a Generative Adversarial Network for 2D Nanomaterials: Implications for Wafer-Scale Semiconductor Characterization

Chun Zhou

Fine-tuning of universal machine-learning interatomic potentials for 2D high-entropy alloys

Selective defect creation in 2D hexagonal boron nitride via ultra-low energy Ar ion irradiation

S. Chokappa[1,2] M. Längle[1,3] V. Zobač[1] D. Propst[1,2] T. Susi[1] J. Kotakoski[1]

[1]University of Vienna, Faculty of Physics, Boltzmanngasse 5, 1090 Vienna, Austria
[2]University of Vienna, Vienna Doctoral School in Physics, Boltzmanngasse 5, 1090 Vienna, Austria
[3]Univ. Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 91405, Orsay, France

In recent years, point defects in hexagonal boron nitride (hBN) have received increasing attention for being excellent hosts for single photon emitters (SPE) at room temperature [1,2]. SPEs are a growing research area with potential applications in quantum communication and information technology, quantum simulations, as well as photonics [3], which introduces the question of whether defect creation in hBN can be controlled. So far, no conclusive results have been reported correlating the exact defect structure and the quantum emission [4,5]. According to simulations using time dependent density functional theory (TDDFT), an Ar^{+1} ion in a head-on collision with nitrogen requires 34.5 eV to successfully knock it out from the hBN lattice, and 45.5 eV to successfully knock out a boron atom, indicating the possibility of selective defect creation in hBN.In this experimental study, freestanding monolayer hBN samples were prepared using the electrochemical delamination method and subjected to 150 eV Ar^{+1} ion irradiation. Using our interconnected ultra-high vacuum system [6], the irradiation effects were directly characterized via scanning transmission electron microscopy (STEM) without exposing the samples to ambient conditions. With the help of a semi-automated STEM image acquisition tool [7], built into our microscope's software, thousands of atomic resolution images of the hBN samples were acquired before and after the irradiation. The acquired images were then analyzed by a semi-autonomous convolutional neural network (CNN) that can identify the hBN lattice, vacancies, and substitutions, giving us an understanding of the defect types and their distributions. By irradiating with an energy higher than the defect creation energy for both boron and nitrogen, we find a surprising result where the ratio between the defects are not equal but have a significant difference that cannot be explained by simulations.From the analysis, the as-prepared samples have an intrinsic defect density of 0.023 nm^{-2} with a roughly 1:1 ratio in B:N single vacancies, but ca. 40% of the boron single vacancies were found to be filled by Si atoms. After irradiation, we found a defect density of 0.243 nm^{-2} with a roughly 85:15 ratio in B:N single vacancies and respective 3:1 and 6:1 ratio of single-to-double and single-to-triple vacancies. We also observe that many vacancies have been filled by Si and C

atoms. Overall, we show a high defect creation probability at this ion energy and demonstrate that such irradiation already provides selectivity in the defect types created.

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High-Performance Mixed-Dimensional Reconfigurable Field-Effect Transistors with Enhanced Polarity Control

A. Echresh[1] S. Ghosh [1] M. Khan [1] P. Chava [1] K. Watanabe [3] T. Taniguchi [3] S. Prucnal [1] R. Hübner [1] Y. Georgiev [1] A. Erbe [1,2]

[1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), 01328 Dresden, Germany
[2]Technische Universität Dresden, Centre for Advancing Electronics (CfAED), 01069 Dresden, Germany
[3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

The continued physical downscaling of CMOS technology is approaching fundamental limits, motivating the exploration of alternative device concepts and material platforms. One promising approach is the reconfigurable field-effect transistor (RFET), which can be dynamically programmed to exhibit n- or p-type behavior through electrostatic control [1]. In this work, we present a novel mixed-dimensional RFET concept based exclusively on one-dimensional (1D) silicon (Si) nanowires integrated with two-dimensional (2D) materials [2]. The device architecture consists of intrinsic Si nanowires contacted with nickel (Ni), followed by annealing to form silicided regions. The resulting silicide–Si interfaces create Schottky junctions, whose carrier injection properties are modulated by appropriate gate architectures. Ambipolar transport is achieved via electrostatic control using back-gate or top-gate configurations. The primary objective of this study is the optimization of Si nanowire RFETs employing hexagonal boron nitride (hBN) as a 2D dielectric and encapsulation layer instead of conventional thermally grown oxide. Owing to its atomically smooth surface, absence of dangling bonds, chemical stability, and dielectric constant comparable to SiO_2, hBN represents a suitable gate dielectric for nanoscale devices. Top-down fabrication of the Si nanowires is carried out using electron beam lithography and reactive ion etching [3], while controlled formation of silicided Schottky junctions is achieved by flash-lamp annealing [4]. Mechanically exfoliated hBN flakes (5–10 nm), characterized by atomic force microscopy and transmission electron microscopy, are transferred onto the devices using a dry viscoelastic stamping technique. Cross-sectional energy-dispersive X-ray spectroscopy confirms the element distribution. Electrical characterization demonstrates enhanced ambipolar and unipolar transfer characteristics and a significant improvement in subthreshold swing for hBN-encapsulated Si RFETs, particularly under top-gate operation, highlighting the effectiveness of 2D dielectric integration in mixed-dimensional silicon-based reconfigurable devices [5].

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Quantifying the detectability of surface defects in $CuInS_2$ quantum dots through DFT-informed electron microscopy simulations

A. Edvardsen[1] J. R. Jinschek[1]

[1]Technical university of Denmark, Kongens Lyngby, Denmark

Surface defects in semiconductor nanocrystals, such as reconstructions, vacancies, and adatoms, govern structural and electronic properties, and thereby their overall functionality. In $CuInS_2$ (CIS) quantum dots (QDs), these defects induce only subtle local lattice distortions that lie at the limits of what electron microscopy can detect, leaving a key question unanswered: Under what imaging conditions do these distortions become experimentally visible? Here, first-principles calculations are combined with electron microscopy (EM) image simulations to evaluate the detectability of surface defects in CIS QDs under experimentally relevant conditions. Representative CIS surface defect motifs are generated and relaxed using density functional theory (DFT). The resulting structures serve as the basis for multislice simulations of EM imaging modalities, including HR-TEM/HR-STEM and diffraction-based approaches such as 4D-STEM. Using a practical experimental parameter space, including accelerating voltage, probe size, convergence angle, detector geometry, and realistic electron dose limits corresponding to low signal-to-noise ratios, we calculate quantitative performance criteria for defect detection. By directly comparing pristine and defect-containing surface structures and quantitatively evaluating both real-space image contrast and reciprocal-space signatures, we generate a matrix of detectability describing the conditions under which subtle structural distortions in CIS QDs become experimentally resolvable. This matrix will allow for the selection of imaging modes that maximize sensitivity to specific defect classes at electron dose levels compatible with radiation-sensitive QDs. The result is a transferable, DFT-informed approach for predicting detection limits prior to experiments, providing clear guidance for the selection of imaging techniques and acquisition strategies when investigating subtle surface distortions in semiconductor quantum dots.

Determining Energy Dispersion of Spin Excitations with Scanning Tunneling Spectroscopy

J. Henriques[1] C. Zhao[2] G. Catarina[2] P. Ruffieux[2] R. Fasel [2]
J. Fernández-Rossier[1]

[1]International Iberian Nanotechnology Laboratory, Braga, Portugal
[2]EMPA, Dübendorf, Switzerland

Conventional methods to measure the dispersion relations of collective spin excitations involve probing bulk samples with particles such as neutrons, photons, or electrons, which carry a well-defined momentum. Open-ended finite-size spin chains, on the contrary, do not have a well-defined momentum due to the lack of translation symmetry, and their spin excitations are measured with an eminently local probe, using inelastic electron tunneling spectroscopy (IETS) with a scanning tunneling microscope (STM). Here[1], we discuss under what conditions STM-IETS spectra can be Fourier-transformed to yield dispersion relations in these systems. We relate the success of this approach to the degree to which spin excitations form standing waves. We show that STM-IETS can reveal the energy dispersion of magnons in ferromagnets and triplons in valence bond crystals, but not that of spinons, the spin excitations in Heisenberg spin-1/2 chains. We compare our theoretical predictions with state-of-the-art measurements on nanographene chains that realize the relevant spin Hamiltonians.

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Linking Alkali Distribution and Mn Redox Gradients in Manganese Oxide Nanocrystals: A Combined STEM-EELS and First-Principles Study

P. Indyka[1] K. Górecki[3] J. Gryboś[3]

[1]Jagiellonian University, National Synchrotron Radiation Centre SOLARIS, Kraków, Poland
[2]Jagiellonian University, Faculty of Chemistry, Kraków, Poland
[3]Jagiellonian University, Faculty of Chemistry, Kraków, Poland

Understanding how cation distribution governs electronic structure and morphology in transition-metal oxides remains a key challenge in the rational design of catalytic materials. In this work, we combine scanning transmission electron microscopy with electron energy-loss spectroscopy (STEM-EELS) and first-principles calculations (density functional theory, DFT) to establish structure-property relationships in two model manganese oxides: tunnel-structured $K_2Mn_8O_{16}$ and layered $Na_2Mn_3O_7$.The materials were synthesized via precipitation, hydrothermal, and solid-state routes, enabling systematic variation of precursors, stoichiometry, and thermal treatment. The STEM-EELS spectrum imaging at the Mn $L_{2,3}$ and O-K edges provides spatially resolved insight into Mn valence states and Mn–O hybridization within individual nanocrystals. Quantitative analysis of white-line ratios, edge onset shifts, and ELNES features reveals pronounced nanoscale redox heterogeneity, including surface-to-core gradients and site-specific variations correlated with alkali ion distribution.Correlative high resolution STEM and EDX mapping show that crystal morphology (nanorods in $K_2Mn_8O_{16}$ and platelets in $Na_2Mn_3O_7$) directly reflects the underlying crystallographic framework and governs cation localization.Complementary DFT calculations, combined with ab initio thermodynamics, were used to determine stable surface terminations, morphology, and oxygen vacancy formation energies. For the most stable structural models, computed electronic structure descriptors were directly compared with EELS energy-loss near-edge structures, enabling a consistent interpretation of spectral features in terms of local coordination and oxidation states. By integrating multi-scale spectroscopy with atomistic modeling, this study establishes a mechanistic link between alkali distribution, defect chemistry, and redox behavior in manganese oxide nanocrystals. The results highlight the predictive power of first principles approaches in interpreting experimental spectra and guiding the design of oxide catalysts for thermochemical applications.Acknowledgements: The research is carried out within the OPUS 25 (grant number 2023/49/B/ST4/00740, PI: dr Joanna Gryboś) project, funded by NCN, the Polish National Science Centre.

Tip recognition in NC-AFM images in liquid

F. Irandoost[1] F. Federici Canova[2] T. Dickbreder[3] F. Sabath[4] T. Fukuma[5] A. Kühnle[6] A. Foster[1,5]

[1]Department of Applied Physics, Aalto University; Espoo 02150, Finland
[2]Nanolayers Research Computing Ltd., London NW9 6PL, England
[3]Department of Physical Chemistry, University of Vienna, Vienna, Austria
[4]Department of Physics at Interfaces Max Planck Institute for Polymer Research, Germany
[5]Nano Life Science Institute (WPI-NanoLSI), Kanazawa University; Kanazawa 920-1119, Japan
[6]Physical Chemistry I, Bielefeld University, Bielefeld, Germany

In-liquid NC-AFM imaging of periodic crystals, such as calcite, often reveals varying hydration patterns, although the sample remains unchanged. These variations arise from factors like tip and imaging height [1,2], and while expert eyes can distinguish between them, there is a gap for a systematic and quantitative approach.In the current study, firstly, we developed an algorithm to extract features from such periodic patterns using Fourier transforms (FT). While FT provides a solid mathematical background to analyze ideal periodic patterns, practical challenges—such as noise in the data and low resolution—must be tackled. After establishing FT-based descriptors, we implemented a workflow for automated pattern recognition, leveraging Equivariant Steerable CNNs[3,4] and clustering algorithms for large calcite datasets.In this work, we present our method to utilise FT-based analysis for describing calcite patterns in NC-AFM data. Our tool offers extensive processing and correction options, allowing experimentalists to adjust analyses depending on their data or application. It also reduces the computational demands, enabling the automated recognition of patterns in large image datasets. In the end, we will present current findings from the analysis of hydration patterns on different surfaces to identify the tip.

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Atomically clean free-standing two-dimensional materials through heating in ultra-high vacuum

P. Irschik[1,2] D. Lamprecht[1,3] S. Chokappa[1,2] C. Mangler[1] C. Speckmann[1] T. A. Bui[1,2] M. Längle[1] L. Filipovic[3] J. Kotakoski[1]

[1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria
[2]Vienna Doctoral School in Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria
[3]Institute for Microelectronics, TU Wien, Gußhausstraße 27-29/E360, 1040 Vienna, Austria

Surface contamination not only influences but in some cases even dominates the measured properties of two-dimensional (2D) materials. Although different cleaning methods are often used for contamination removal, commonly used spectroscopic cleanliness assessment methods can leave the level of achieved cleanliness ambiguous. Therefore, despite two decades of research on 2D materials, the true cleanliness of the used samples is often left open to interpretation. While cleaning procedures for graphene have been extensively employed and studied[1], there is a lack of reporting on the cleaning of monolayer hexagonal boron nitride, particularly at the atomic level, despite its despite its various projected applications, such as being a dielectric for nanoelectronic devices, and for quantum information and sensor technology due to its quantum light emission across a wide spectral range. In this work, free-standing monolayer graphene and hexagonal boron nitride are annealed at different temperatures in a custom-built ultra-high vacuum heating chamber, connected to a scanning transmission electron microscope via a vacuum transfer line[2], enabling atomically resolved cleanliness characterization as a function of annealing temperature, while eliminating the introduction of airborne contamination during sample transport. We find that, while annealing at 200°C already reduces contamination significantly, it is not until 400°C or higher, where over 90% of the free-standing monolayer areas are atomically clean. At this point, further contamination removal is mainly limited by defects in the material and metal contamination introduced during the sample transfer or growth. In addition, we find annealing-induced defects to be negligible in quantity, which provides the pristine, atomically clean areas necessary for further structural manipulations, such as defect or pore creation through more controlled techniques like electron or ion irradiation[3,4].

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The effects of noble gas intercalation on bilayer MoS_2 sheets: A DFT study

P. James[1] E. H. Åhlgren[1]
[1]University of Helsinki

2D MoS_2 is a material of significant interest because its electronic band structure and catalytic activity can be tuned by modifying layer thickness or introducing structural defects such as strain and vacancies in the lattice. This opens interesting possibilities for creating new MoS_2-systems with targeted properties. This work investigates the effects of noble gas (He, Ar, Xe) intercalation on bilayer MoS_2 using ab initio density functional theory (DFT) simulations with the Quantum Espresso software package. We investigate bilayer supercells of varying dimensions (1×1, 2×2, 3×3, and 4×4) each containing a single intercalated noble gas atom, resulting in systems with different noble gas densities between the layers. The electronic band gap structure is resolved for each system and compared against pristine bilayer (indirect bandgap of ∼1.6eV) and monolayer MoS_2 structures (direct bandgap of ∼1.9 eV) [1]. The results indicate that noble gas intercalation causes the bandgap of bilayer MoS_2 to approach that of pristine monolayer MoS_2 as supercell size increases and noble gas atomic density decreases. Furthermore, the bandgap in all intercalated systems is indirect, consistent with the behavior observed in all pristine MoS_2 structures thicker than a monolayer. There is a notable exception with the 3×3×2 systems, in which noble gas intercalation produces a direct bandgap regardless of the noble gas species.

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Atomic-Scale Assembly of Quantum Defects in Two-Dimensional Semiconductors with the Scanning Tunneling Microscope

D. Jansen[1] G. Miao[1] J. Keienburg[1] J. Beckmann[1] J. Fischer[1] T. Michely[1] H. Komsa[2] W. Jolie[1]

[1]Institute of Physics II, University of Cologne, Cologne, Germany
[2]Faculty of Information Technology and Electrical Engineering, University of Oulu, Oulu, Finland

Point defects in two-dimensional (2D) semiconductors hold great potential for quantum technologies, such as spin-qubits or single-photon emitters [1-3] and many candidates have been theoretically identified in the past. However, controlled experimental realization and characterization remains challenging, as it requires creation of well-defined structures embedded in an otherwise pristine material.

Here we present how the scanning tunneling microscope (STM) can be employed to fabricate, characterize and manipulate single point defects and defect complexes on the atomic scale in the 2D semiconductors MoS_2 and WS_2. With the help of transition metal adatoms that are evaporated onto the 2D materials at low temperature [4], we create basal plane substitutional defects M_S, in which a single sulfur atom is replaced by the transition metal. A special focus lies on the Mo_S antisite defect in MoS_2, which is predicted to host a spin triplet ground state that could serve as a spin qubit [1, 2]. In WS_2 we create sulfur vacancies that are assembled into vacancy complexes by making use of a sulfur atom diffusion process induced by inelastic tunneling. Some of these complexes are predicted to be bright color centers, depending on the underlying symmetry [3]. Scanning tunneling spectroscopy is employed to characterize the emergent hybrid in-gap states of the various complexes. Density functional theory calculations are instrumental in interpretation of the experimental results and provide insight into the electronic structure of the defects. Emergent opportunities in the field of single spin control of atomic defects in 2D semiconductors created by STM are demonstrated in recent experiments [5].

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From four t(w)o three: An exploration of interferometric 4D-STEM for measuring 3D variations in twisted bilayer graphene

C. Kofler[1,2] F. Libisch[3] T. Susi[1] J. Kotakoski[1]

[1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria
[2]Vienna Doctoral School in Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria
[3]Institute for Theoretical Physics, TU Vienna, Wiedner Hauptstrasse 8-10/136, 1040 Vienna, Austria

Four-dimensional (4D) scanning transmission electron microscopy (STEM) has become an almost routine procedure in high-level electron microscopy due to the combination of modern pixelated direct-electron detectors and computers able to handle the massive resulting diffraction data. However, computational power is merely the muscle, and requires solid theory and steadfast thought behind the employed analysis. Therefore, a lot of effort has gone into developing ways to coax novel information from 4D-STEM datasets. While some methods, like ptychography or center of mass imaging, are by now well established, others remain challenging. Here, we discuss interferometric 4D-STEM, a method still in its adolescence, that could shed light on a property well hidden from conventional STEM, the three-dimensional (3D) structure of thin specimen, in particular twisted bilayer graphene. There, the overlap of the identical but twisted layers leads to the formation of periodic moiré patterns, superstructures that cause the periodic modulation of various properties such as the distance between the layers, which varies depending on the local stacking order [1].Interference patterns formed in the overlap regions of convergent-beam diffraction disks originating from the separate layers when probed with a defocused beam contain information on the subtle interlayer distance variations. Careful analysis could thus provide a spatially resolved distance map over the whole moiré pattern. Building upon the works by Latychevskaia [2] and Zachman [3], who established the foundation of this method, we examine whether, to what extent, with which resolution, and under what conditions interferometric 4D-STEM yields sensible results, by systematically testing it against simulated data of increasing complexity.This systematic study aims to lay the groundwork for future experimental work and provide a useful starting point for people interested in doing similar work. With the nature of data and also of science itself changing in the wake of technological advances, it is more important than ever to share our work and support one another in our quest for good, reliable, and open research.

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Advancing scanning probe microscopy simulations: A decade of development in probe-particle models

N. Oinonen[1,2] A. V. Yakutovich[3,4] A. Gallardo[5] M. Ondracek[6] P. Hapala[6] O. Krejci[1,7]

[1]Department of Applied Physics, Aalto University, P.O. Box 11000 (Otakaari 1B), AALTO, FI-00076, Finland
[2]Nanolayers Research Computing Ltd, 51 New Way Road, London, NW9 6PL, United Kingdom
[3]nanotech@surfaces laboratory, Swiss Federal Laboratories for Materials Science and Technology (Empa), Überlandstrasse 129, Dübendorf, CH-8600, Switzerland
[4]National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Lausanne, CH-1015, Switzerland
[5]IMDEA Nanoscience Institute, C/ Faraday 9, Campus de Cantoblanco, Madrid, 28049, Spain
[6]Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, Prague 8, 182 00, Czech Republic
[7]Department of Chemistry and Material Science, Aalto University, P.O. Box 11000 (Otakaari 1B), AALTO, FI-00076, Finland

Since its inception more than a decade ago [1], the probe particle model has become an important tool for simulating high-resolution SPM images obtained with flexible tip apices, shedding light on the origin of the contrast patterns observed in experiments. Our recent review [2] discusses the development of the probe particle simulations over the years, with emphasis on the open source ppafm package for AFM simulations [3]. Starting from a simple model utilizing a Lennard-Jones force field, ppafm has expanded to include various force field models for electrostatic and Pauli interactions utilizing data from ab initio calculations, as well as other simulation modes including STM and KPFM. The GPU acceleration has sped up the simulations by 2-3 orders of magnitude, allowing for development of machine learning tools for SPM image interpretation [4]. Finishing with a graphical user interface making the package more user friendly and easier to approach. At the very end, I will shortly introduce my current project on recovering surface reconstruction with a help of machine learning and scanning probe microscopy simulations.

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Structure and Properties of Mirror-Twin Boundary Networks in Substoichiometric $MoTe_2$: Insights from First-Principles Calculations

D. Kruklinskii[1] M. Ghorbani-Asl[1] A. V. Krasheninnikov[1]

[1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Defect engineering in two-dimensional (2D) materials offers a powerful route to emergent electronic phases beyond those accessible in pristine crystals. The experiments [1] demonstrate that in substoichiometric $MoTe_2$, point defects condense into extended mirror-twin boundaries (MTBs) that self-organize into periodic networks, forming a homologous series of novel crystalline phases. Scanning tunneling microscopy reveals that these phases consist of periodically arranged triangular MTB loops, while our density functional theory calculations show that the experimentally observed structures lie on or near the convex hull, providing a unified thermodynamic framework for their stability. The preferred structural motif arises from energetically favorable vertex configurations and specific relative offsets between MTB domains. Electronic structure calculations further demonstrate that these ordered MTB networks give rise to Kagome-like flat bands with pronounced Van Hove singularities, and in certain cases, emergent ferromagnetism. These findings establish MTB phases not as mere defect arrangements but as distinct 2D crystals with tunable quantum properties. Our results highlight a general strategy for engineering correlated electronic states through defect ordering in low-dimensional materials.

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Moiré Plane Wave Expansion Model

M. Le Ster[1] K. Palotás[2] P. Vancsó[1] P. Kowalczyk[3] P. Nemes-Incze[1]

[1]HUN-REN Centre for Energy Research, Konkoly-Thege Miklós út 29-33, 1121 Budapest, Hungary
[2]HUN-REN Wigner Research Centre for Physics, Konkoly-Thege Miklós út 29-33, 1121 Budapest, Hungary
[3]University of Lodz, ul. Pomorska 149/153, 90-236 Lodz, Poland

Simulating twisted van der Waals multilayer systems can be computationally very demanding, especially as the twist angle decreases due to the large number of atoms in the supercell. In this work, we introduce the energy- and height-dependent Moiré Plane Wave Expansion Model (MPWEM) which only requires the charge density data of the individual non-interacting two-dimensional material - that may be obtained by density functional theory (DFT) calculations - and uses its Fourier components to construct the charge density of the interacting multilayer system. With only a small number of intuitive parameters, such as the coupling strength between the component layers and screening, we can reconstruct the charge density of the interacting system with very good approximation. We illustrate the model with twisted bilayer graphene and $MoTe_2$/graphene moiré systems. This method can also be applied to incommensurate systems which lack translational symmetry as verified by experimental scanning tunneling microscopy in a variety of systems [1,2].

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Molecular Hamiltonian learning from setpoint-dependent scanning tunneling spectroscopy

G. Lupi[1] A. O. Fumega[1] M. Amini[1] R. Drost[1] P. Liljeroth[1] J. Lado[1]

[1]Department of Applied Physics, Aalto University, 02150 Espoo, Finland

Molecular quantum magnets adsorbed on surfaces exhibit rich spin and orbital excitations that can be probed by scanning tunneling microscopy with inelastic electron tunneling spectroscopy (STM-IETS). However, the quantitative extraction of the underlying multiorbital Hamiltonian from experimental spectra remains a fundamental challenge. Here, we introduce molecular Hamiltonian learning, a machine learning strategy that infers the microscopic Hamiltonian parameters of a single adsorbed molecule directly from the setpoint-dependence of STM-IETS data. The method leverages the systematic evolution of spectral features as the STM tip tunes the local electrostatic environment for different tip-sample distances. We demonstrate this approach on iron phthalocyanine on ferroelectric SnTe, training our algorithm on theory spectra from a realistic multiorbital model, including spin-orbit coupling, electrostatic interactions, local crystal field, and substrate effects. The algorithm, trained solely on theoretical many-body simulations, allows reconstructing Hamiltonian parameters directly from experimental spectra. Our manuscript establishes a flexible and automated strategy for Hamiltonian reconstruction from STM-IETS, transforming setpoint-dependent spectroscopy into quantitative characterization of quantum materials at the atomic scale.

Ultra-low energy ion irradiation of few-layer MoS2: defect production and intercalation

R. Nawaz[1] P. James[1] B. Maria Mayer[2,4] J. Kotakoski[4] K. Mizohatal[1] A. Lopez Cazalilla[3] E. Åhlgren[1,2,4]

[1]Department of Physics, University of Helsinki, 00560 Helsinki, Finland.
[2]Department of Physics and Astronomy, University of Uppsala, SE-751 20 Uppsala, Sweden.
[3]Barcelona Supercomputing Center, Placa Eusebi Guell 1-3, 08034 Barcelona, Spain.
[4]Faculty of Physics, University of Vienna, 1090 Vienna, Austria.

Two-dimensional (2D) materials such as molybdenum disulfide (MoS_2) and other transition-metal dichalcogenides (TMDs) have attracted significant interest due to their unique electronic, optical, and mechanical properties [1]. These materials show great potential for applications in electronics, optoelectronics, catalysis, and energy storage. However, their applications often require wafer-scale manufacturing going beyond current growth-based capabilities. Ion implantation is a powerful approach for top-down modification of materials by introducing controlled defects and dopants [2]. However, the reduced dimensionality of 2D materials poses restrictions for their nanofabrication and requires ion beams to operate at very low energies, from some hundreds of eV to a few tens of eV. The ultra-low energy manufacturing of 2D TMDs is not yet fully understood.In this work, the effects of ultra-low-energy argon and xenon ion implantation on MoS_2 are studied using scanning transmission electron microscopy, Raman spectroscopy, and molecular dynamics simulations. Mechanically exfoliated MoS_2 samples were irradiated with the KIIA ion accelerator at the University of Helsinki at doses of 1×10^{14} to 1×10^{15} ions/cm^2 with ion energies ranging from 15 to 200 eV. Structural analysis shows pore-type defect formation, while MD simulations reveal that the onset of defect generation in MoS_2 begins at ∼35–40 eV for Ar, with sulfur sputtering exhibiting a stepwise increase above $\sim 1 \times 10^{14}$ cm^{-2}, while at lower fluences the increase is more gradual; a similar but less pronounced trend is observed for Mo. These nonlinear sputtering effects are more pronounced for Xe and emerge at lower ion energies compared to Ar, intensifying as the ion energy increases. At higher energies, reaching 60 eV for Xe, both S and Mo sputtering rise rapidly around $\sim 5 \times 10^{14}$ cm^{-2}, indicating accelerated defect accumulation and membrane de-stabilization. This behavior is consistent with previous Ga ion irradiation studies of MoS_2, where low fluences primarily increased pore density while higher fluences ($\sim 10^{14}$ cm^{-2}) led to vacan-cy coalescence and growth of larger nm-scale pores [3]. The simulations further reveal an intermediate energy window where ions can be trapped between MoS_2 layers. However, at high ion

fluence, the trapped ions may escape through nm-sized pores that form when defects coalesce.

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Tip-enhanced Raman Spectroscopy simulation methods

P. Planelles Prensa[1] A. Ghafoor[2] H. Sethi[1] O. Jose Silveira[1] A. Foster[1]
[1]Aalto University, Department of Applied Physics
[2]University of Jyvaskyla

Tip-enhanced Raman Spectroscopy (TERS) has emerged as a promising technique that overcomes Abbe diffraction limit, which dictates that for green light around 500 nm the spatial resolution is limited to only 250 nm, which is insufficient for studying nanomaterials. In TERS, by using a strongly localized plasmonic field produced at the tip apex, the Raman signal is significantly enhanced, and submolecular resolution can be achieved.Similar to Scanning Tunneling and Atomic Force Microscopy techniques, TERS relies on a sharp tip. TERS offers the additional advantage of providing not only topographic information about the sample, but also chemical.Despite the rapidly increasing interest in TERS, progress remains limited by the difficulty of interpreting the resulting experimental images.In this context, we aim to contribute by presenting ab-initio simulation methods and demonstrating how they can be used to greatly facilitate the interpretation and prediction of TERS images. Moreover, we will study the influence of the substrate on the images, and how different tip geometries and materials affect resolution and induce image asymmetry. We will also compare several simulation methods with different levels of complexity and computational cost.

Orbital Ordering in 2D Multiferroic VCl3/HOPG

A. Puzari[1] L. Camerano[2] A. O. Fumega[1] J. Lado[1] P. Liljeroth[1] S. Ganguli[1]

[1]Department of Applied Physics, Aalto University School of Science, P.O. Box 15100, 00076 Aalto, Finland

[2]Department of Physical and Chemical Sciences, University of L'Aquila, Via Vetoio, 67100 L'Aquila, Italy

Orbital ordering in two-dimensional van der Waals (vdW) materials can give rise to exotic symmetry-broken phases. However, direct experimental evidence of orbital-ordered states has remained largely elusive. Monolayer (ML) VCl_3, a magnetic vdW material, has been theoretically predicted to host an orbital-ordered phase that breaks the intrinsic C_3 symmetry of the lattice, inducing structural distortion in the chlorine sublattice, and giving rise to ferroelectricity [1].In this work, we grow ML-VCl_3 on highly oriented pyrolytic graphite (HOPG) using molecular beam epitaxy and investigate its electronic structure using a scanning tunneling microscope (STM). By directly mapping the local density of states (LDOS) of the top-layer chlorine atoms, we visualize the electronic density of the underlying orbital ordering of vanadium atoms. Comparison with theoretical calculations indicates the presence of an antiferro-orbital ordered phase in ML-VCl_3.Interestingly, we observe that the symmetry-broken ferroelectric ground state can be tuned by an external magnetic field, where the C_2-symmetric state reverts to the undistorted C_3 symmetry phase beyond a critical field. We further perform a detailed study of ferroelectric domains within the symmetry-broken phase. Our measurements reveal pronounced band bending at ML-VCl_3 island edges and weaker band bending along domain boundaries, consistent with their ferroelectric origin. In addition, we demonstrate local manipulation of these ferroelectric domains via the tip-induced electric field and observe temperature-dependent changes in domain orientation.Together, these findings establish ML-VCl_3 as a field-tunable multiferroic vdW magnet and provide direct experimental evidence that orbital ordering acts as the primary symmetry-breaking mechanism. This work opens pathways toward symmetry-switchable electronics and orbitally engineered quantum functionalities in two-dimensional materials.

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Ferroelectric relaxation dynamics of twisted bilayer hexagonal boron nitride

N. Stenbrink[1] P. Hernandez-Leon[2] A. O. Fumega[1] T. Antao[1] J. L. Lado[1] M. A. Caro[2]

[1]Department of Applied Physics, Aalto University
[2]Department of Chemistry and Materials Science, Aalto University

2D van der Waals heterostructures is a fascinating group of materials, due to the control and tunability of properties. This can be done in multiple ways, but a relatively new way of tuning these materials is twisting of a layer. Examples of the effect of twisting include superconductivity in graphene and ferroelectricity in hexagonal boron nitride [1, 2].There is a relatively new theory of sliding ferroelectricity, in which sliding in xy-plane leads to a polarization in z-direction [3]. Effectively this perturbation in xy-plane can be seen to lead to a distortion of the pz-orbital, i.e., the charge distribution in that direction. Rotation (or twisting) and sliding are similar enough that this could be a part of the explanation for the emerging polarization.Studying the lattice dynamics of this system is crucial to understanding the material properties. Here we study the relaxation displacements and phonons (lattice vibrations) in order to gain more information on material, keeping the transition from insulating to ferroelectric phase, that results from twisting, in mind.

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Multilayer Van der Waals Heterostructures: Opportunities Beyond the 2D Limit

P. Sutter[1] E. Sutter[2]

[1]Department of Electrical & Computer Engineering, University of Nebraska-Lincoln
[2]Department of Mechanical & Materials Engineering, University of Nebraska-Lincoln

Heterostructures of two-dimensional (2D) crystals have attracted broad interest due to novel properties that arise as atomically thin materials are stitched laterally or stacked vertically. Potentially as interesting scientifically and technologically, but much less explored are synthetic heterostructures between few-layer or multilayer van der Waals crystals. Major challenges exist in growth, doping, controlled interface formation, and the probing of emerging properties of such layered heterostructures at the relevant (nanometer) scale.Here, we discuss recent research that addresses these challenges by combining microscopy of growth and processing with advanced materials characterization and spectroscopy of optoelectronics at the ultimate resolution limit. We focus on group IVA monochalcogenides, MX (where M = Ge, Sn; X = S, Se), an emerging class of isostructural layered semiconductors with bandgaps between 0.9 – 1.6 eV. Lateral heterostructures combining multilayer SnS/GeS or SnS/GeSe show stunning interface control with atomically sharp layer-by-layer connectivity across hundreds of individual van der Waals layers [1–3]. Combined cathodoluminescence spectroscopy and ab-initio calculations shed light on carrier transfers and charge separation at such lateral interfaces. Doping of MX semiconductors has been a long-standing issue due to ubiquitous self-doping by native point defects. Overcoming this problem through controlled substitutional doping has paved the way for the realization of electrically active pn-junctions in lateral heterostructures [4]. In vertical heterostructures, new opportunities arise for valleytronics via valley-selective carrier transfers across planar van der Waals interfaces [5], and for templating ferroelectric order between different MX crystals [6]. Our results highlight the rich functionalities that can be realized in both lateral and vertical van der Waals heterostructures beyond the 2D limit.

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Macroscopic Tin Monochalcogenide Van der Waals Ferroelectrics: Growth, Alloys, Doping, Domain Structures, and Curie Temperatures

E. Sutter[1] P. Sutter[2]

[1]Department of Mechanical and Materials Engineering, University of Nebraska-Lincoln, USA
[2]Department of Electrical and Computer Engineering, University of Nebraska-Lincoln, USA

2D and layered van der Waals crystals present opportunities for creating new families of ferroelectrics with switchable electric polarization, elastic strain, or magnetic order at thicknesses down to the single-layer limit. So far, synthesis was limited to small (few microns) crystals, where proximity to edges affects domain patterns and severely limits the ability to fabricate complex device architectures required for accessing functionalities in van der Waals ferroelectrics. Here, we report the realization of in-plane ferroelectric few-layer crystals of the monochalcogenides tin(II) sulfide, selenide, and sulfoselenide (SnS, SnSe, $SnSe_{1-x}S_x$) whose linear dimensions exceed the current state of the art by an order of magnitude [1-3]. Such large crystals allow the investigation of ferroelectric domain patterns that are unaffected by edges and finite size effects. Analysis by in-situ transmission electron microscopy and nanobeam diffraction determines the characteristics of the ferroelectric phase across the $SnSe_{1-x}S_x$ system [1-3], provides measurements of Curie temperatures [2,4], and sheds light on symmetry breaking and the transition between the polar and the symmetric (high-T) phase [4]. Finally, we demonstrate controlled n-type doping of the Sn monochalcogenide crystals, which in pure state show invariably p-type conductivity. The combined results highlight a new class of van der Waals ferroelectrics with promise for energy conversion, information storage, and novel computing paradigms.

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Tuning the Kondo temperature of MoS_2 mirror twin boundaries on graphene

T. Tounsi[1] K. Vyas[1] C. van Efferen[1] G. Miao[1] A. Safeer[1] A. Karaka[1] A. Rosch[2] J. Fischer[1] T. Michely[1] T. Costi[3] W. Jolie[1]

[1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany
[2]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany
[3]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

Mirror twin boundaries (MTBs) are one-dimensional line defects that exhibit a Kondo effect [1,2]. It was shown that this effect arises from confining a spin $\frac{1}{2}$ along the boundary, which is screened by the bath electrons. The $\mathrm{d}I/\mathrm{d}V$ signatures of the Kondo effect in monolayer MoS_2 MTBs are the zero-bias resonance peak, in addition to a singly occupied state below the Fermi level E_F and a doubly unoccupied state above E_F [1]. The experimental data give access to the Anderson model parameters: the splitting U of the non-degenerate states, the impurity orbital's position ε with respect to E_F, and the impurity level's bare width γ_0.In this work, we compare the Kondo temperature (T_K) measured in MTBs of MoS_2 grown on three different substrates. In the case of MoS_2 / Graphene (Gr) / Ir(111), T_K was in the range $[10^{-4}\,\mathrm{K}, 10^{-10}\,\mathrm{K}]$ [1]. By intercalating a single layer of Eu under Gr, we noticed a decrease in γ_0, leading to a drop in T_K. In the third system, MoS_2 / Gr / Ir(110), T_K increased significantly to the range $[1\,\mathrm{K}, 10\,\mathrm{K}]$. This enabled us to study the Kondo effect at the boundary between the weakly screened magnetic state above T_K and the Kondo singlet state below T_K.

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Spin Screening in MoS_2 Mirror Twin Boundaries on graphene on Ir(110)

K. Vyas[1] T. Tounsi[1] C. Van Efferen[1] G. Miao[1] A. Safeer[1] A. Karaka[1]
A. Rosch[2] J. Fischer[1] T. Michely[1] T. A. Costi[3] W. Jolie[1]

[1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany
[2]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany
[3]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

Mirror twin boundaries (MTBs) are line defects that host confined states in the bandgap of monolayer MoS_2. The confined states closest to the Fermi energy split into a singly and a doubly occupied level separated by the Coulomb repulsion U, forming a spin-$1/2$ system. The spin of the singly occupied state is then screened by the electron bath present in the substrate below, giving rise to a Kondo resonance pinned to the Fermi energy (1).In this work, we investigate spin screening in MoS_2 MTBs grown on graphene/Ir(110) using low-temperature scanning tunnelling microscopy and spectroscopy. STM imaging reveals well-defined MTBs, while STS spectra recorded along the boundaries show two pronounced impurity peaks separated by the Coulomb energy U, together with a zero-bias feature which can be attributed to the Kondo resonance.Compared to MTBs in MoS_2/Gr/Ir(111) (1), MTBs in MoS_2/Gr/Ir(110) exhibit much higher Kondo intensity and significantly broadened impurity-level widths, indicating strong hybridization γ with the electron bath provided by the graphene/Ir(110) substrate. This enhanced hybridization results in a Kondo temperature (T_K) comparable to the measurement temperatures (0.4 K–7 K), enabling the study of the phase transition between the Kondo singlet phase below and the magnetic phase above the Kondo temperature.

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Microscopic Image Deblurring by a Generative Adversarial Network for 2D Nanomaterials: Implications for Wafer-Scale Semiconductor Characterization

X. Dong[1] Y. Zhang[2]

[1]Institute for Measurement Systems and Sensor Technology, Technical University of Munich
[2]School of Chemical Engineering, Aalto University

Wafer-scale two-dimensional (2D) semiconductors with atomically thin layers are promising materials for fabricating optic and photonic devices. Bright-field microscopy is one of the most efficient methods for large-area characterization and quality control. However, a significant challenge is the focus drift that occurs during long scanning processes, which results in blurred images and limits the accuracy of automated analysis.To address this, we propose a deep learning approach to restore these out-of-focus images. We developed a Generative Adversarial Network (GAN) using a combined loss function (MS-SSIM and L1) to effectively recover both structural details and color fidelity. Our results show that the model achieves a high structural similarity index (SSIM $>$ 90%) compared to the ground truth. Furthermore, by using these restored images for segmentation, we were able to automatically identify monolayer and multilayer regions with over 80% accuracy. This work demonstrates that machine learning can be a practical solution to overcome hardware limitations in the microscopic characterization of 2D nanomaterials.

Fine-tuning of universal machine-learning interatomic potentials for 2D high-entropy alloys

C. Zhou[1] H. P. Komsa[1]

[1]Microelectronics Research Unit, Faculty of Information Technology and Electrical Engineering, University of Oulu, P.O. Box 4500, Oulu, FIN-90014, Finland

High-entropy alloys (HEAs) and their two-dimensional counterparts have attracted increasing interest due to their tunable properties and catalytic potential, while their chemical complexity poses significant challenges for first-principles modeling. In this work, we discuss our recent progress on combining density functional theory (DFT) and universal machine-learning interatomic potentials (uMLIPs) to study two-dimensional transition metal sulfide HEAs. We assess the applicability of several leading uMLIPs and show that direct use of universal models is insufficient for reliably describing key energetic quantities such as mixing energies. We then present effective fine-tuning strategies based on systematically generated random and enumerated structures, which substantially improve model robustness and accuracy. We validate the fine-tuning strategies across three distinct structural databases constructed from different alloy configurations, showing that enumeration-based training sets generally lead to more efficient and stable models compared to random structure selection. Using the experimentally synthesized (Mo,Ta,Nb,W,V)S_2 system as a case study, we integrate the fine-tuned models with Monte Carlo simulations to analyze phase decomposition behavior and observe phase separation behavior that follows the temperature-dependent Gibbs free energy trends of the quinary alloy and its possible decomposition products. Overall, the study demonstrates the potential of fine-tuned uMLIPs for modeling chemically complex alloys, while emphasizing the importance of carefully designed training strategies for achieving reliable predictions.

Participants

Amato Michele	France	michele.amato@universite-paris-saclay.fr
Bellani Vittorio	Italy	vittorio.bellani@unipv.it
Brihuega Ivan	Spain	ivan.brihuega@uam.es
Chokappa Shrirang	Austria	shrirang.chokappa@univie.ac.at
Echresh Ahmad	Germany	a.echresh@hzdr.de
Edvardsen Albert Elias Tronholm	Denmark	altroe@dtu.dk
Fernández Rossier Joaquín	Portugal	joaquin.fernandez-rossier@inl.int
Fischer Jeison	Germany	jfischer@ph2.uni-koeln.de
Foster Adam	Finland	adam.foster@aalto.fi
Ghaderzadeh Sadegh	United Kingdom	sadegh.ghaderzadeh@nottingham.ac.uk
Ghorbani-Asl Mahdi	Germany	mahdi.ghorbani@hzdr.de
Indyka Paulina	Poland	paulina.indyka@uj.edu.pl
Irandoost Farzin	Finland	farzin.irandoost@aalto.fi
Irschik Philipp	Austria	philipp.irschik@univie.ac.at
James Patrick	Finland	patrick.james@helsinki.fi
Jansen Daniel	Germany	jansen@ph2.uni-koeln.de
Javed Umair	Austria	umair.javed@univie.ac.at
Klein Julian	United States	jpklein@mit.edu
Kofler Clara	Austria	clara.kofler@univie.ac.at
Komsa Hannu-Pekka	Finland	hannu-pekka.komsa@aalto.fi
Krasheninnikov Arkady	Finland	arkady.krasheninnikov@aalto.fi
Krejci Ondrej	Finland	ondrej.krejci@aalto.fi
Kruklinskii Daniil	Germany	dan261299@gmail.com
Lado Jose	Finland	jose.lado@aalto.fi
Le Ster Maxime	Hungary	le.ster.maxime@ek.hun-ren.hu
Lehenkari Touko	Finland	lehenkari.touko@gmail.com
Louie Steven	United States	sglouie@berkeley.edu
Lupi Greta	Finland	greta.lupi@aalto.fi
Längle Manuel	France	manuel.langle@universite-paris-saclay.fr
Mayer Barbara Maria	Sweden	barbara.maria.mayer@physics.uu.se
Meunier Vincent	United States	vincent.meunier@psu.edu
Michely Thomas	Germany	michely@ph2.uni-koeln.de
Nawaz Rabia	Finland	rabia.nawaz@helsinki.fi
Okuno Hanako	France	hanako.okuno@cea.fr
Palotas Krisztian	Hungary	palotas.krisztian@wigner.hu
Planelles Prensa Pablo	Finland	pablo.planellesprensa@aalto.fi
Puzari Animesh	Finland	animesh.puzari@aalto.fi
Stenbrink Nils Henrik Samuli	Finland	nilshenriksamuli.stenbrink@aalto.fi
Suenaga Kazu	Japan	suenaga-kazu@sanken.osaka-u.ac.jp
Susi Toma	Austria	toma.susi@univie.ac.at

Sutter Peter	United States	psutter@unl.edu
Sutter Eli	USA	esutter@unl.edu
Tounsi Tfyeche Y	Germany	tounsi@ph2.uni-koeln.de
Tran Tuan	Sweden	tuan.tran@physics.uu.se
Unterleutner Elena	Austria	elena.unterleutner@tugraz.at
Vyas Kuber	Germany	vyas@ph2.uni-koeln.de
Zhang Yucheng	Finland	yucheng.zhang@aalto.fi
Zhou Chun	Finland	czhou24@univ.yo.oulu.fi