

# Towards Reality in Nanoscale Materials X

12th – 14th February 2019  
Levi, Finland





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# Programme

	Tuesday	Wednesday	Thursday
8:45	<i>Intro</i> <i>chair: Blum</i>	<i>chair: Schluger</i>	<i>chair: Kotakoski</i>
9:00	<b>Neugebauer</b>	9:00 <b>Blum</b>	9:20 <b>Arenal</b>
9:40	<b>Kühnle</b>	9:40 <b>Zanolli</b>	10:00 Georgiev
10:20	Tocci	10:20 Achilli	10:20 Schnorr
10:40	<i>Coffee</i>	10:40 <i>Coffee</i>	10:40 <i>Coffee</i>
	<i>chair: Kuhnle</i>	<i>chair: Tkatchenko</i>	<i>chair: Zanolli</i>
11:20	<b>Voitchovsky</b>	11:20 <b>Oganov</b>	11:20 <b>Wilhelm</b>
12:00	Schulz	12:00 Hapala	12:00 Ghorbani-Asl
12:20	Huda	12:20 Hofer	12:20 Popov
12:40	Ilie	12:40 Caro	12:40 Strand
13:00	<i>Lunch</i>	13:00 <i>Lunch</i>	13:00 <i>Lunch</i>
16:40	<i>Coffee</i>	16:40 <i>Coffee</i>	16:40 <i>Coffee</i>
	<i>chair: Oganov</i>	<i>chair: Wilhelm</i>	<i>chair: Neugebauer</i>
17:00	<b>Shluger</b>	17:00 <b>Meyer</b>	17:00 <b>Maier</b>
17:40	Todorova	17:40 <b>Smet</b>	17:40 <b>Tkatchenko</b>
18:00	McKenna	18:20 Kotakoski	18:20 Kantorovitch
18:20	Pellegrin	18:40 Posters	
		21:00 <i>Dinner</i>	

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# Tuesday 12.02.2019

- 8:45 - 9:00 *Intro*  
*chair: Blum*
- 9:00 - 9:40 **Neugebauer**  
Extending First-Principles Calculations to Model Electrochemical Reactions at the Solid-Liquid Interface
- 9:40 - 10:20 **Kühnle**  
Hydration layer mapping on mineral surfaces
- 10:20 - 10:40 **Tocci**  
On slip and diffusion of water confined between two-dimensional materials from ab initio molecular dynamics
- 10:40 - 11:20 *Coffee*
- chair: Kuhnle*
- 11:20 - 12:00 **Voitchovsky**  
Probing the dynamics of single molecules at solid-liquid interfaces: an experimental perspective
- 12:00 - 12:20 **Schulz**  
Insights into complex natural processes from high-resolution atomic force microscopy
- 12:20 - 12:40 **Huda**  
Epitaxial ferromagnetic VSe<sub>2</sub> monolayers on superconducting NbSe<sub>2</sub>
- 12:40 - 13:00 **Ilie**  
Defects in WSe<sub>2</sub> and WSe<sub>2</sub>/metal heterostructures investigated by Quasi-Particle Interference mapping and STM/STS
- 13:00 - 16:40 *Lunch*
- 16:40 - 17:00 *Coffee*
- chair: Oganov*
- 17:00 - 17:40 **Shluger**  
Role of Carrier Injection and Localization in Degradation of Oxide Films
- 17:40 - 18:00 **Todorova**  
Ab initio description of oxides in electrochemical environment by constructing defect and surface phase diagrams
- 18:00 - 18:20 **McKenna**  
Electronic properties of extended defects in solar absorbers
- 18:20 - 18:40 **Pellegrin**  
Dynamic highly coloured Copper(I) - bis(diimine) coordination polymer: an efficient and innovative photocatalyst

## Extending First-Principles Calculations to Model Electrochemical Reactions at the Solid-Liquid Interface

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Many of the technological challenges we presently face, such as improving battery materials, electrocatalysis, fuel cells, or corrosion protection, originate from reactions at solid-liquid electrochemical interfaces. Describing and quantifying the underlying fundamental mechanisms is challenging both for experimental and theoretical techniques. Combining concepts from semiconductor physics and corrosion science, we have developed a novel approach that allows us to perform ab initio calculations under controlled potentiostat conditions for electrochemical systems. The proposed approach can be straightforwardly applied in standard density functional theory codes and allows to obtain direct insight into key mechanisms of electrocatalysis and corrosion such as water splitting, H<sub>2</sub> evolution, desorption of surface atoms, solvation etc. To show the performance and the opportunities opened by this approach we discuss several prototypical examples: Corrosion at the water- Mg interface [1], dissolution of Mg under anodic polarization and structure formation at the standard hydrogen electrode.

[1] S. Surendralal, M. Todorova, M. Finnis und J. Neugebauer, *Phys. Rev. Lett.* **120**, 246801 (2018).

## Hydration layer mapping on mineral surfaces

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Solid-liquid interfaces are omnipresent both in nature and technology. In geochemistry, many processes are governed by the structure and reactivity of the involved interfaces [1]. Likewise, understanding biomineralization for biomimetic materials design will require elucidating the fundamental steps in nucleation and growth at the interface [2]. Recent advances in dynamic atomic force microscopy (AFM) have opened up the possibility to resolve the solvation structure at solid-liquid interfaces [3]. In this talk, we will present improvements in AFM instrumentation that allow for three-dimensional solvation layer mapping [4]. Using this technique, interfacial cations can be identified [5] and defect sites can be resolved by their hydration structure [6]. These insights will be important for gaining a molecular-level understanding of the structure and reactivity of solid-liquid interfaces.

[1] A. Putnis, *Science* **343**, 1441 (2014).

[2] A.S. Schenk, *Adv. Funct. Mater.* **22**, 4668 (2012).

[3] T. Fukuma, Y. Ueda, S. Yoshioka, H. Asakawa, *Phys. Rev. Lett.* **104**, 016101 (2010).

[4] H. Söngen, M. Nalbach, H. Adam, A. Kühnle, *Rev. Sci. Instrum.* **87**, 063704 (2016).

[5] H. Söngen, C. Marutschke, P. Spijker, E. Holmgren, I. Hermes, R. Bechstein, S. Klassen, J. Tracey, A.S. Foster, and A. Kühnle, *Langmuir* **33**, 125 (2017).

[6] H. Söngen, B. Reischl, K. Miyata, R. Bechstein, P. Raiteri, A.L. Rohl, J.D. Gale, T. Fukuma, A. Kühnle, *Phys. Rev. Lett.* **120**, 116101 (2018).

## On slip and diffusion of water confined between two-dimensional materials from ab initio molecular dynamics

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Water slip under confinement has received increased attention in the recent years, driven by the interest to develop efficient desalination membranes, as well as nanoscale osmotic power generators [1,2]. The electronic and chemical nature of materials has been suggested to be highly relevant to slip [3,4]. In this work, we present results on the structure and collective dynamics (i.e. the friction and the diffusion coefficient of the fluid) of liquid water confined between graphene, hBN, and MoS<sub>2</sub> sheets from ab initio molecular dynamics simulations. We find that the friction coefficient changes dramatically between the three materials, due to their strikingly different underlying energy landscape. We also report on an intriguing mechanism driving slip under confinement, where stronger confinement regimes give rise to an enhanced slip, due to a reduced friction decorrelation time. Finally, we find that the mean square displacement of the liquid under confinement may not be linear with time (as it is instead in Brownian motion), and instead its exponent may depend on the confining material.

[1] Siria A, Bocquet ML, Bocquet L. , *Nature Reviews Chemistry* **1**, 11 (2017).

[2] Abraham J, Vasu KS, Williams CD, Gopinadhan K, Su Y, et al. , *Nature Nanotechnology* **12**, 546 (2017).

[3] Tocci G, Joly L, Michaelides A., *Nano Letters* **14**, 6872 (2014).

[4] Secchi E, Marbach S, Niqués A, Stein D, Siria A, Bocquet L., *Nature* **537**, 210 (2016).

## Probing the dynamics of single molecules at solid-liquid interfaces: an experimental perspective

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The motion of liquid molecules and solutes at the interface with solids underpins countless processes from heterogenous catalysis to crystal growth, self-assembly and the function of biomembranes. Experimentally, probing the dynamics of single molecules at interfaces remains challenging due to highly localised interactions between the molecules and the surface of the solid. Typical approaches based on spatial and temporal averaging often fail to capture key local information. Atomic force microscopy (AFM) can in principle overcome this issue, especially when complemented by computational approaches. AFM has been used successfully to probe the detailed molecular arrangements of numerous solid-liquid interfaces at equilibrium. Measurements of the dynamics of single molecules at interfaces are however still sparse due to limited time resolution. Recent work [1] has shown that the unusual properties of the interfacial liquid can considerably slow down interfacial dynamics [2] potentially enabling AFM investigation in suitable systems. In this presentation I will review some of our recent results in the field, in particular the implications of interfacial molecules' dynamics for the function of biomembranes [3] and in lubrication processes [4].

[1] M. Ricci, P. Spijker, K. Voitchovsky, *Nature Commun.* **5**, 4400 (2014).

[2] M. Ricci, W. Trewby, C. Cafolla, K. Voitchovsky, *Sci. Rep.* **7**, 43234 (2017).

[3] L. Piantanida, H. Bolt, N. Rozatian, S. Cobb, K. Voitchovsky, *Biophys. J.* **113**, 426 (2017).

[4] C. Cafolla, K. Voitchovsky, *Nanoscale* **10**, 11831 (2018).

## Insights into complex natural processes from high-resolution atomic force microscopy

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Many processes in nature are based on the formation and growth of large organic molecules from basic building blocks, their subsequent transformation or agglomeration and in some cases, their decomposition or oxidation. Examples for such processes are pyrolysis, soot formation in combustion, the cycling of dissolved organic carbon in the ocean and the formation of crude oil.

On the atomic scale, these are highly complex phenomena, which often involve diverse mixtures of molecules. Knowledge of the chemical structure of individual molecular constituents yields valuable insights into the chemistry of such processes. Unfortunately, deriving chemical structures from techniques such as mass spectrometry or nuclear magnetic resonance is not straightforward, in particular for larger molecules or diverse mixtures.

Atomic force microscopy with CO-functionalized tips (CO-AFM) [1] has recently demonstrated the capability to identify chemical structures of individual compounds in complex mixtures of unknown molecules [2]. Here, we apply CO-AFM to analyze molecular mixtures of various origins and demonstrate how chemical structure elucidation leads to valuable insights on the reaction pathways of important chemical processes of nature.

[1] L. Gross et al., *Science* 325, 1110 (2009).

[2] B. Schuler et al., *J. Am. Chem. Soc.* 137, 9870 (2015).

## Epitaxial ferromagnetic VSe<sub>2</sub> monolayers on superconducting NbSe<sub>2</sub>

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Combination of magnetism and superconductivity has been predicted to result in a novel phase of matter called topological superconductivity. This has recently attracted intense interest due to the predicted boundary modes hosting Majorana fermions and their relevance to topological quantum computation. Topological superconductivity has been experimentally realized in 1D in both engineered nanowire systems and in chains of magnetic adatoms on a superconducting substrate [1,2]. Very recently, these concepts have been extended to 2D by studying the edge modes around magnetic islands on superconducting substrates [3-5]. However, these systems are sensitive to the atomic scale details of the coupling between the magnetic layer and the substrate and in some cases, require interface engineering using an atomically thin separation layer. This creates a big challenge in real device applications and there clearly is a need for more robust experimental systems for the realization of 2D topological superconductivity.

We propose a new platform based on the recently discovered 2D monolayer van der Waals ferromagnet vanadium diselenide (VSe<sub>2</sub>) that can be grown directly on layered materials [6]. Here, we report the growth of monolayer VSe<sub>2</sub> by molecular beam epitaxy (MBE) on superconducting niobium diselenide (NbSe<sub>2</sub>) substrate. We characterize the electronic and magnetic properties by low-temperature scanning tunneling microscopy (STM) and macroscopic magnetization measurements. The demonstration of the coexistence of ferromagnetism and superconductivity in a hybrid van der Waals heterostructure will provide opportunities for the investigation of novel quantum phases of matter and open new possibilities for real-life device applications.

- [1] Vincent Mourik, *Science* 336, 1003-1007 (2012).
- [2] Stevan Nadj-Perge, *Science* 1259327, 1259327 (2014).
- [3] Joel Röntynen, *PhysRevLett.* 114, 236803 (2015).
- [4] Gerbold C Menard, *Nature communications* 8, 2040 (2017).
- [5] Alexandra Palacio-Morales, *arXiv preprint* 1809, 04503 (2018).
- [6] Manuel Bonilla, *Nature Nanotechnology* 13(4), 289 (2018).

## Defects in WSe<sub>2</sub> and WSe<sub>2</sub>/metal heterostructures investigated by Quasi-Particle Interference mapping and STM/STS

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Defects in transition metal dichalcogenides (TMDs) are local atomic modifications which can affect the electronic and magnetic properties of the material. Here we focus on WSe<sub>2</sub> which is one of the semiconducting TMDs and has great potential in both spintronics and valleytronics.

We studied defects in WSe<sub>2</sub> crystals and monolayers by scanning tunnelling microscopy and spectroscopy (STM/STS), coupled with quasi-particle interference (QPI) mapping, at 4K and 77K. Among a large variety of defect configurations, we identified a few that based on QPI appear to support spin-flip processes. We have also studied monolayers of WSe<sub>2</sub> on atomically flat metallic surfaces and used QPI from defects to characterize such heterostructures and band structure modifications.



## Role of Carrier Injection and Localization in Degradation of Oxide Films

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Most current electronic and electrochemical devices are stacks of thin films and interfaces operating under electrical stress. Nanometre-thick oxide films play crucial role in performance of these devices. Injection of excess electrons and holes into oxide films is responsible for the mechanisms that govern the formation of conductive filaments in resistance switching memory devices, the dielectric breakdown in microelectronic devices, and the performance of photo-electrochemical and oxide fuel cells. Our theoretical modelling combined with experimental observations demonstrates that structural disorder in amorphous  $\text{SiO}_2$ ,  $\text{Al}_2\text{O}_3$ ,  $\text{TiO}_2$ ,  $\text{ZnO}$  and  $\text{HfO}_2$  films creates precursor sites which can spontaneously trap up to two electrons or holes in deep states in the band gap. The results demonstrate that single- and bi-polaron electron and hole states can form in a-  $\text{SiO}_2$  [1] and a-  $\text{HfO}_2$  [2] where the effect of local disorder is amplified by polaronic relaxation of amorphous network. Only hole trapping is found in a- $\text{Al}_2\text{O}_3$  [3] The electron localization weakens Me-O bonds, which can be broken upon thermal activation, creating an  $\text{O}^{2-}$  interstitial ion and a neutral O vacancy [4].  $\text{O}^{2-}$  interstitial ions can easily diffuse through the oxide and in devices are guided to the positive electrode by the electric field [5]. Multi-scale modelling [6] including electron injection rates, defect creation and electron hopping rates through created defects is used to describe dielectric breakdown in oxide films. The results demonstrate that the creation and field-driven movement of oxygen ions causes changes in oxide structure on a much larger scale than previously thought.

[1] A.-M El-Sayed et al., *Phys. Rev. B* **89**, 125201 (2014).

[2] M. Kaviani et al., *Phys. Rev. B* **94**, 020103 (2016).

[3] O. Dicks et al., *J. Phys.: Condens. Matter* **29**, 314005 (2017).

[4] D. Z. Gao et al., *Nanotechnology* **27**, 505207 (2016).

[5] A. Mehonic et al., *Adv. Mater.* **28**, 7486 (2016).

[6] A. Padovani et al., *J. Appl. Phys.* **121**, 155101 (2017).

## Ab initio description of oxides in electrochemical environment by constructing defect and surface phase diagrams

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Electrochemistry offers a huge number of possibility to tune materials properties desired in the context of practical problems such as water electrolysis and batteries, electro-catalysis, photo-catalytic water splitting or corrosion. The quantitative description of materials behaviour presents, however, challenges because of the involvement of different length scales, time scales and materials classes. Our recently developed unifying approach for semiconductor defect chemistry and electrochemistry [1] naturally links ab initio calculations to experimental observables such as  $pH$  and electrode potential  $U$ , enabling us to characterise materials properties in electrochemical environment. One way in which we can utilize the approach is the construction of relevant Pourbaix-type diagrams, which enable us to discuss the stability of an oxide and its surface reconstructions in electrochemical environment, i.e. against  $pH$  and  $U$ . Two examples will be presented. Defect Pourbaix diagrams revealing the dominant point defects governing the growth and dissolution of the oxide barrier layer forming when Zn comes into contact with a corrosive environment [2]. Surface Pourbaix diagrams showing stable surface reconstructions forming on the polar Zn-terminated ZnO(0001) surface and which reveal the that solvation effects are substantial, highly selective and play an active role in shaping the surface [3, 4].

[1] M. Todorova and J. Neugebauer, *Phys. Rev. Applied.* **1**, 014001 (2014).

[2] M. Todorova and J. Neugebauer, *Faraday Discuss.* **180**, 97 (2015).

[3] S. Yoo, M. Todorova und J. Neugebauer, *Phys. Rev. Lett.* **120**, 066101 (2018).

[4] S. Surendralal, M. Todorova, M. Finnis und J. Neugebauer, *Phys. Rev. Lett.* **120**, 246801 (2018).

## Electronic properties of extended defects in solar absorbers

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Thin-film solar absorber materials promise high efficiencies together with low-cost and are actively pursued for next generation solar cell technologies [1]. Although all emerging materials are multicomponent and polycrystalline little is currently known about the role of extended defects and associated point defect segregation [2]. To provide insight into these issues we perform first principles theoretical predictions of the electronic properties of highly stable extended defects in several next generation solar absorber materials. These include 111 twin boundaries in pure formamidinium lead iodide (FAPbI<sub>3</sub>); a mixed ion lead halide perovskite containing formamidinium, Cs, I and Br; and a 1/2[110](001) anti-site boundary (ASB) in Cu<sub>2</sub>ZnSnSe<sub>4</sub> (CZTSe).

We find the 111 twin boundary in pure FAPbI<sub>3</sub> is extremely stable but introduces no electron or hole trapping states and presents relatively small barriers (< 100 meV) to transport of electrons and holes, suggesting they are relatively benign for solar cell performance [3]. However, in the mixed ion perovskite twin boundaries serve as a nucleation site for formation of an I- and Cs-rich secondary phase. The reduced band gap in this segregated phase leads to hole trapping and is likely to enhance electron-hole recombination and lead to reduced open circuit voltage in solar cell devices. The 1/2[110](001) ASB in CZTSe is also highly stable but like pure FAPbI<sub>3</sub> does not present a recombination site or current blocking layer, so that photovoltaic device performance is not significantly degraded [4]. Altogether, these results provide atomistic insight into the properties of stable extended defects in solar absorbers and highlight the role they can play as nucleation sites for secondary phases which can be extremely detrimental to solar cell performance.

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[2] D. W. de Quilettes et al, *Science* **348**, 683 (2015).

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[4] B. Mendis et al, *J. Mater. Chem. A* **6**, 189 (2018).

## Dynamic highly coloured Copper(I) – bis(diimine) coordination polymer: an efficient and innovative photocatalyst

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Ruthenium polypyridine complexes epitomized by  $[\text{Ru}(\text{bpy})_3]^{2+}$ , feature well-known outstanding properties such as a strong absorption in the visible and long-lived excited states. As such, they dominate the world of coordination compounds photochemistry despite their toxicity and cost. Copper(I)-diimine complexes  $[\text{Cu}(\text{L})_2]^+$  (L = diimine such as 1,10-phenanthroline) are very intriguing alternatives to ruthenium compounds. Indeed, they display very similar spectroscopic features to  $[\text{Ru}(\text{bpy})_3]^{2+}$  (broad absorption band at ca. 460 nm, MLCT character). Importantly, they are a) luminescent and b) can drive photochemical reactions such as water reduction[1,2] or organic photochemical transformations[3]. The lability of the copper(I)-diimine coordination sphere is however a matter of concern: ligand scrambling is a rather favoured phenomenon with those complexes. They are thus easily degraded by de-coordination in presence of concurrent ligands, thus limiting the lifetime of the corresponding photosystems[4]. Aiming at stabilizing the latter, we propose to synthesize a dynamic coordination polymer CP1 and use the self-healing properties of such species to increase the stability of the rather fragile copper(I) chromophores in photocatalytic conditions. In this contribution, we will report the full characterization of the CP1 polymer based on a ditopic tetrapyridophenazine ligand, substituted by butyl chains in alpha of the chelating nitrogen atoms. We notably report its exceptional photochemical behaviour in presence of a variety of substrates.

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[2] S. Fischer; D. Hollmann; S. Tschierlei; M. Karnahl; N. Rockstroh; E. Barsch; P. Schwarzbach; S.-P. Luo; H. Junge; M. Beller; S. Lochbrunner; R. Ludwig; A. Brueckner, *ACS Catal.* **4**, 1845 (2014).

[3] A. C. Hernandez-Perez; S. K. Collins, *Acc. Chem. Res.* **49**, 1557 (2016).

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# Wednesday 13.02.2019

- chair: Schluger*
- 9:00 - 9:40 **Blum**  
All-electron theory of new inorganic and organic-inorganic semiconductors
- 9:40 - 10:20 **Zanolli**  
Spintronics at the interface
- 10:20 - 10:40 **Achilli**  
Ge- $V_n$  complexes in silicon: a viable route toward room temperature quantum information
- 10:40 - 11:20 *Coffee*
- chair: Tkatchenko*
- 11:20 - 12:00 **Oganov**  
Computational Materials Discovery Using Evolutionary Algorithm USPEX
- 12:00 - 12:20 **Hapala**  
Computer aided AFM imaging and recognition of 3D molecules
- 12:20 - 12:40 **Hofer**  
An Extended Electron Approach to the General Many-Body Problem
- 12:40 - 13:00 **Caro**  
Machine learning local atomic properties within the Gaussian approximation potential framework
- 13:00 - 16:40 *Lunch*
- 16:40 - 17:00 *Coffee*
- chair: Wilhelm*
- 17:00 - 17:40 **Meyer**  
Graphene hybrids and extended defects: Revealing 3D structures, dynamics, and new insights to radiation damage
- 17:40 - 18:20 **Smet**  
Ultrafast diffusion and superdense ordering of lithium ions in the single van der Waals gap of bilayer graphene
- 18:20 - 18:40 **Kotakoski**  
Scanning transmission electron microscopy of air-sensitive samples and under controlled low-pressure atmospheres
- 18:40 - 21:00 **Posters**
- 21:00 - 23:00 *Dinner*

## All-electron theory of new inorganic and organic-inorganic semiconductors

V. Blum<sup>1</sup>

<sup>1</sup>Department of Mechanical Engineering and Materials Science and Department of Chemistry, Duke University, Durham, NC, USA

This talk describes some recent progress in our group regarding accurate, efficient all-electron approaches in computational simulations of new inorganic and organic-inorganic materials. We first cover recent progress in the FHI-aims all-electron code and in the open-source infrastructure "ELSI" for efficient, parallel simulations of materials with large system sizes using current, massively parallel supercomputing resources. Specific applications covered include joint experiment-theory work on the discovery of new defect resistant ternary chalcogenide semiconductors I2-II-IV-IV4 (e.g., Cu<sub>2</sub>BaSn(S,Se)<sub>4</sub>), as well as tunable organic-inorganic hybrid perovskite semiconductors including large, optically active organic components.

This overview talk covers joint work with many colleagues, including the groups of David Mitzi (Duke), Yosuke Kanai (UNC), Matthias Scheffler (FHI Berlin), Xinguo Ren (USTC Hefei), group members at Duke University, and the very large developer community of the FHI-aims code. Part of this work was supported by the National Science Foundation (CBET-1511737, DMR-1729297) and the US Department of Energy (CHOISE EFRC).

## Spintronics at the interface

Z. Zanolli<sup>1</sup>

<sup>1</sup>Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Spain

The interface between materials can be considered as the ultimate spintronics device, not only in terms of miniaturization but also to unlock unique design possibilities and new physical properties which are unattainable in the individual bulk materials. As device dimensions are constantly shrinking, understanding the physical properties emerging at interfaces is crucial to exploit them for applications.

Graphene and magnetoelectric multiferroics are promising materials for spintronic devices with high performance and low energy consumption. We combine the features of both materials by investigating from first principles and Monte Carlo simulations the interface between graphene and BaMnO<sub>3</sub>, a magnetoelectric multiferroic. We show [1] that electron charge is transferred across the interface and magnetization is induced in the graphene sheet due to the strong interaction between C and Mn. A remarkably large proximity induced spin splitting of the Dirac cones ( $\sim 300$  meV) is achieved and doping can make the high-mobility region of the electronic bands experimentally accessible.

Spin-Orbit Coupling calculations reveal that graphene deeply affects the magnetic state of the substrate, down to several layers below the interface, by inducing an overall magnetic softening, and switching the in-plane magnetic ordering from anti- to ferromagnetic. The graphene-BaMnO<sub>3</sub> system presents a Rashba gap 300 times larger than in pristine graphene, leading to a new flavor of Quantum Anomalous Hall effect (QAHE), a hybrid QAHE, characterized by the coexistence of metallic and topological insulating states. These findings could be exploited to fabricate novel devices that use graphene to control the magnetic configuration of a substrate [2].

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## Ge- $V_n$ complexes in silicon: a viable route toward room temperature quantum information

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The development of on-demand individual deep impurities in silicon is motivated by their employment as a physical substrate for qubits [1], nanoscale transistors [2] and Hubbard-like quantum systems [3]. Single-atom silicon devices based on conventional doping elements such as phosphorous [4], arsenic [5] and boron, as well as other shallow-level dopants can operate only at cryogenic temperature due to their shallow weakly localized ground state impurity levels [6]. Differently, the implantation of Ge dopants in silicon and the subsequent annealing is expected to generate stable Germanium-vacancy defects [7] that are promising candidates to achieve single-atom quantum effects at room temperature.

These hybrid complexes combine indeed the properties of the silicon vacancy, which carries deep states in the bandgap, with the accurate spatial controllability of the defect obtainable through state of the art single-ion implantation of Ge atom.

By means of ab initio Density Functional Theory (DFT) calculation with screened-exchange hybrid functional, that solves the "gap and delocalization problem" of standard DFT, we characterize structural and electronic properties of different Ge- $V_n$  defects. The calculated thermodynamic charge transition levels, corresponding to the excitation energies for the addition of electrons to the defect, are in very good agreement with the available experiments. Accordingly the electrons are more localized than in conventional dopants decaying in a radius of about 0.5 nanometers from the defect [8].

By mapping the ab initio DFT results in an extended Hubbard formalism, the resonant tunneling in an array of Ge- $V_n$  complexes in silicon is analyzed in order to shed light on the transport mechanisms observed in the experimental I-V curves.

This strongly correlated system is characterized by very large on-site repulsion  $U$  and small electronic hopping  $t$  ( $U/t \sim 250$ ) and can be a platform to study the Mott transition and the antiferromagnetic correlation at half filling.



This study is part of a joined theoretical and experimental project funded by the Horizon 2020 European Funding Programme [9].

- [1] J. J. Pla et al., *Nature* **489**, 541 (2012).
- [2] T. Shinada et al., *Nanoelectronics Workshop (SNW)* , 1-2 (2014).
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- [9] NFFA-EUROPE, *Nanoscale Foundries and Fine Analysis* **Project ID 188 and 517**, (2017-2018).

## Computational Materials Discovery Using Evolutionary Algorithm USPEX

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In the last decade, a number of approaches made it possible to discover new materials on the computer – prior to experimental verification. This holds a transformative potential for the development of new technologies. A special role in this development is played by our evolutionary algorithm USPEX, developed by me and my students since 2006. The methodology will be reviewed along with applications to several problems of materials science.

To enable discovery of technologically useful materials, we implement multiobjective (Pareto) optimization and apply it to a variety of problems: Our new method, Mendeleevian Search, capable of finding the best materials among all possible compounds with all possible crystal structures, will be described and its results illustrated.

I will describe results of our recent works along several lines: 1. Search for novel thermoelectric materials, where we show the possibility of achieving the figure of merit  $ZT \gg 1$ . 2. Discovery of novel superhard materials. 3. Prediction of new high-temperature superconductors. 4. Prediction of novel chemistry of nanoparticles and possible explanation of carcinogenicity of oxide dust.

Current limitations and future prospects of these methods will be discussed.

## Computer aided AFM imaging and recognition of 3D molecules

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In recent decade Atomic Force Microscopy with tip functionalized by carbon monoxide (CO) provided unique tool to experimentally image sub-molecular details of individual organic molecules [1], which is of great importance e.g. for on-surface chemistry. Most experiments are, however, up to now limited to flat aromatic molecules, due to difficulties with interpretation of highly distorted AFM images originating from non-planer molecules due to mechanical relaxation of tip or sample. These problems can be partially overcome using a simple mechanical model (Probe-Particle Model [2]) which can reproduce those distortions, therefore simulate AFM images for given molecular structure. However, this still requires laborious search for molecular structure which reproduces that particular experimental image. Instead we attempt to develop automatic tool to conduct inverse task – to recover molecular structure from given set of AFM images. Preliminary results suggest that convolutional neural network (CNN) [3] trained on simulated AFM images can learn this inverse mapping rather easily. Yet application of the method on real experimental data, and identification of atomic species remains to be a challenge.

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## An Extended Electron Approach to the General Many-Body Problem

T. Pope<sup>1</sup> W. Hofer<sup>1</sup>

<sup>1</sup>School of Physical and Environmental Sciences, Newcastle University

An extended electron model fully recovers many of the experimental results of quantum mechanics while it avoids many of the pitfalls and remains generally free of paradoxes [1]. The formulation of the many-body electronic problem there resembles the Kohn–Sham formulation of standard density function theory. However, rather than referring electronic properties to a large set of single electron orbitals, the extended electron model uses only mass density and field components, leading to a substantial increase in computational efficiency. To date, the Hohenberg–Kohn theorems have not been proved for a model of this type, nor has a universal energy functional been presented. In this paper, we address this problem and show that the Hohenberg–Kohn theorems do also hold for a density model of this type thus paving the way for the development of fast, efficient, and accurate codes on this basis.

[1] Thomas Pope, Werner Hofer, *Frontiers of Physics* 12, 128503 (2017).

## Machine learning local atomic properties within the Gaussian approximation potential framework

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<sup>1</sup>Department of Electrical Engineering and Automation, Aalto University, Finland

<sup>2</sup>Department of Applied Physics, Aalto University, Finland

Molecular dynamics (MD) simulations are a useful tool to understand the interactions between atoms and to get insight into the processes that take place at the nanoscale and give rise to the observed properties of materials. "Classical" interatomic potentials, based on i) harmonic description of bonds, ii) partial electrostatic charges and iii) Lennard-Jones approximations for dispersion interactions, are computationally efficient but do not grant accurate representation of the real underlying physics/chemistry. They tend to fail at flexibly describing molecules in changing environments, especially when there is bond rearrangement, i.e., when chemical reactions take place. Density functional theory (DFT), on the other hand, offers a satisfactory description of interatomic interactions and can be used to characterize bond formation and annihilation. Unfortunately, DFT becomes prohibitively expensive when running MD of systems beyond a few hundreds of atoms or for time scales longer than a nanosecond. To bridge this gap between computational efficiency and accuracy, algorithmic developments that make use of machine learning techniques are being adopted by the community. In particular, the Gaussian approximation potential (GAP) framework [1] is becoming increasingly popular to describe interatomic interactions in the form of cohesive, or "total", energies. However, GAP-type interpolation can be used, in principle, also to learn local atomic properties other than total energies. Adsorption characteristics and spectroscopic signatures of atoms are possibly the most relevant examples. In this presentation, I will introduce a new method to predict adsorption energies, with an example application to amorphous carbon surfaces [2] (although the method is general). I will also present a new type of atomic descriptor which allows us to improve the predictive ability of GAP models and therefore bring them closer to full DFT accuracy [2]. If time allows, I will also discuss ongoing work on machine learning of x-ray spectroscopic signatures within the GAP framework.

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## Graphene hybrids and extended defects: Revealing 3D structures, dynamics, and new insights to radiation damage

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C. Mangler<sup>2</sup> C. Kramberger<sup>2</sup> R. Mirzayev<sup>2</sup> P. Laiho<sup>3</sup> H. Jiang<sup>3</sup> G. Argentero<sup>2</sup>  
V. Skakalova<sup>2</sup> K. Elibol<sup>2</sup> E. I. Kauppinen<sup>3</sup> T. Susi<sup>2</sup> J. Kotakoski<sup>2</sup> J. C. Meyer<sup>1,2</sup>

<sup>1</sup>University of Tübingen, Institute for Applied Physics & Natural and Medical Sciences institute, Germany

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<sup>3</sup>Aalto University School of Science, Department of Applied Physics, Finland

Obtaining the location of every atom in three dimensions is arguably the ultimate goal of electron microscopy. Electron tomography is usually based on a large number of projections, and requires that the sample does not change its structure during data acquisition. Here, we demonstrate that the location of every atom in graphene defects and individual and clustered silicon impurities in graphene can be obtained from only two projections [1,2]. Importantly, two projections could be obtained with no changes in the atomic network, while larger numbers of exposures (e.g. for a complete tomographic series) would be prohibited by the limited radiation stability of the sample. The analysis reveals a kink in the graphene sheet at grain boundaries that depends on the misorientation angle. For 3-coordinated silicon impurities, we could confirm the out-of-plane position of the Si atom from direct images and also follow beam-induced dynamics where the impurity changes from one side of the graphene sheet to the other, in both directions. The 3D structure could also be obtained for a graphene sheet that interacts with cleanly deposited single-walled carbon nanotubes [3]. In this hybrid system, the van der Waals interaction leads to a deformation of both the carbon nanotube and the graphene sheet. Finally, we have studied hybrids of graphene and molecular structures, namely C60 fullerenes [4] and chlorinated copper phthalocyanine (ClCuPc) [5]. They represent the first cases that mono-layers of organic molecules were studied by electron microscopy at atomic resolution. In the graphene-fullerene sandwich, dynamics of entire molecules can be observed with weakly bound fullerenes oscillating between different positions at the edges of 2D C60 molecular crystals. Moreover, we observed the transition from rotating individual fullerenes through dimers with suppressed rotation to molecular clusters locked into position. Atomic resolution studies of ClCuPc mon o-layers on graphene provided new insights to radiation damage. The critical dose of the mono-layers is orders of magnitude lower than that of bulk crystals, and the molecular fragments form cross-linked networks on the graphene surface after the loss of the chlorine atoms.

## Ultrafast diffusion and superdense ordering of lithium ions in the single van der Waals gap of bilayer graphene

J. H. Smet<sup>1</sup> M. Kühne<sup>1</sup> S. Fecher<sup>1</sup> F. Paolucci<sup>1</sup> J. Popovic<sup>1</sup> D. Samuelis<sup>1</sup>  
P. M. Ostrovsky<sup>1</sup> J. Maier<sup>1</sup> F. Börrnert<sup>2</sup> J. Biskupek<sup>2</sup> U. Kaiser<sup>2</sup>  
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Solids that simultaneously conduct electrons and ions are key elements for the mass transfer and storage required in battery electrodes. Single-phase materials with a high electronic and high ionic conductivity at room temperature are hard to come by, and therefore multiphase systems with separate ion and electron channels have been put forward instead. Here we report on bilayer graphene as a single-phase mixed conductor and demonstrate the diffusion of lithium faster than in graphite and even surpassing the diffusion of sodium chloride in liquid water [1]. To measure diffusion of lithium we have developed an on-chip electrochemical cell architecture in which the redox reaction, that forces lithium intercalation, is localized at a protrusion of the device only. This geometry has the advantage of allowing for a well-defined one dimensional diffusion front so the 2D material can be operated as a true single-phase mixed conductor and also leaving the graphene bilayer unperturbed from the electrolyte during operation. Time-dependent Hall measurements across spatially displaced Hall probes enable to monitor the in-plane diffusion kinetics within the single van der Waals gap of the bilayer. The intercalation is reversible.

The device concept with a perimetrial galvanic cell is transferrable to other 2D materials and thin films and the immediate accessibility of the mixed conductor surface also offers the possibility of deploying local probe and surface analysis techniques to study the local kinetics and ordering of an intercalate otherwise hidden underneath the electrolyte. Here, we have chosen to perform transmission electron microscopy even though probing light elements such as lithium ions and carbon atoms is severely hampered by their low scattering cross section for impinging electrons and their susceptibility to knock-on damage. Working at low acceleration voltage becomes crucial, but demands the use of spherical and chromatic aberration correctors to maintain true atomic resolution. We achieve true atomic resolution and contrary to expectation, we observe the formation of a high density, multi-layered crystalline phase of lithium in

between the graphene sheets [2]. The associated lithium storage exceeds by far the densest configuration realized in bulk graphitic carbon under similar conditions.

- [1] M. Kühne, F. Paolucci, J. Popovic, P.M. Ostrovsky, J. Maier, J.H. Smet, *Nature Nanotechnology* **12**, 895 (2017).
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## Scanning transmission electron microscopy of air-sensitive samples and under controlled low-pressure atmospheres

G. T. Leuthner<sup>1</sup> C. Mangler<sup>1</sup> T. Susi<sup>1</sup> J. C. Meyer<sup>2</sup> J. Kotakoski<sup>1</sup>

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<sup>2</sup>University of Tübingen, Germany

Scanning transmission electron microscopy (STEM) is a powerful technique for the study of atomic structure and spectroscopic fingerprints of materials down to the level of individual atoms. However, in typical instruments the samples need to be inserted through air, which makes the study of air sensitive samples difficult with this method. In this contribution, we present first results from the Vienna setup built around a Nion UltraSTEM100 that allows the transfer of samples between external systems and the microscope in an Ar atmosphere. This enables the study of air-sensitive samples that have either been created in a protective atmosphere or made sensitive through treatment for example by energetic ion irradiation.

Additionally, in many instruments, the pressure at the sample during observation is limited to ca.  $1e-7$  mbar, providing a large number of gas molecules for the electron beam to crack, which can lead to structural changes in the sample. Since the exact composition of the gas atmosphere at the sample is unknown, it is difficult to study the role of different gases in the observed dynamic processes. In our setup, through the addition of an all-metal leak-valve to an instrument with a base pressure at the sample on the order of  $1e-10$  mbar, we can directly address this issue. In this presentation, we show the effect of leaked air as well as its constituent gases on the etching of carbon-based contamination on a mono-layer graphene sample. Air, water and oxygen all lead to etching, whereas hydrogen and nitrogen atmospheres have no influence as compared to experiments in ultra high vacuum (UHV). Oxygen provides an etching effect that is two times more efficient than that of water, presumably due to two oxygen atoms per molecule in the oxygen gas. We also show that in UHV, graphene edges with the armchair configuration are stable even under the electron beam, whereas in an oxygen atmosphere they become unstable and only zigzag edges can be imaged. These studies show that controlled low-pressure atmospheres in transmission electron microscopes can be used to carry out chemical modification of materials at the nanometer scale.



# Thursday 14.02.2019

- chair: Kotakoski*
- 9:20 - 10:00 **Arenal**  
Doped Nanodiamonds: Chemical information at the atomic scale via EELS
- 10:00 - 10:20 Georgiev  
Fabrication and Particular Applications of Group IV Semiconductor Nanowires
- 10:20 - 10:40 Schnorr  
Charging dynamics of self-assembled InAs quantum dots in n-GaAs Schottky diodes
- 10:40 - 11:20 *Coffee*
- chair: Zanolli*
- 11:20 - 12:00 **Wilhelm**  
Ultrafast neutralization dynamics of highly charged ions upon impact on 2D materials
- 12:00 - 12:20 Ghorbani-Asl  
Ion beam modification of single-layer transition metal dichalcogenides
- 12:20 - 12:40 Popov  
Enhancing of catalytic activity of MoS<sub>2</sub> single layers through spontaneous oxidation under ambient conditions
- 12:40 - 13:00 Strand  
Point defects in hexagonal Boron Nitride
- 13:00 - 16:40 *Lunch*
- 16:40 - 17:00 *Coffee*
- chair: Neugebauer*
- 17:00 - 17:40 **Maier**  
On-surface assembly and reaction of molecular nanostructures: from metals to insulating surfaces
- 17:40 - 18:20 **Tkatchenko**  
Covalent and Non-Covalent Interactions in Molecular Systems
- 18:20 - 18:40 Kantorovitch  
Kinetic control in molecular self-assembly on an insulating surface

## Doped Nanodiamonds: Chemical information at the atomic scale via EELS

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Chemical analyses at the local (sub-nanometer/atomic) scale are crucial for improving the understanding of materials. For instance, for doped carbon nanostructures (as those of diamond family), these analyses are critical because their properties strongly depend on the chemical environment/configuration of the dopants [1-4]. Electron energy-loss spectroscopy (EELS), developed in an aberration-corrected TEM (having access to a close to 1 angstrom electron probe), is an essential and powerful technique to perform such local chemical analyses [2-4]. In this contribution, we will present a detailed study of the structure and local composition of nitrogen-doped ultrananocrystalline diamond (UNCD) films [5-8]. Under normal process conditions, these UNCD films are highly electrically insulating, but they can become highly conducting when Ar is substituted in the synthesis gas with some of N<sub>2</sub> [1, 4-8]. The formation of these NWs starts to appear when the N<sub>2</sub> content in the gas phase reaches about 10% in volume. From these studies, we concluded that the insulator-metal transition of these films is strongly correlated with the formation of these diamond NWs. Indeed, these NWs are enveloped by a sp<sup>2</sup>-based carbon layer providing the conductive path for electrons [5-8]. In summary, these studies elucidate crucial questions concerning the local composition (atomic configuration) of these materials. This detailed knowledge is essential for better understanding the outstanding properties of such materials.

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## Fabrication and Particular Applications of Group IV Semiconductor Nanowires

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During the last 1-2 decades semiconductor nanowires (NWs) have received significant academic and commercial attention due to their attractive electrical and mechanical properties and large surface area to volume ratios. They have a variety of possible applications including nanoelectronics, nanophotonics, photovoltaics, sensorics, etc. Among all semiconductor NWs the ones based on group IV materials have the advantage of being the most silicon (Si) compatible. This is very important since their integration into the existing semiconductor technology platform can be relatively easy.

We will give a general overview of our activities on group IV nanowires. We will first present the NWs that we are working with, including top-down fabricated Si and germanium (Ge) NWs having widths down to 6-7 nm as well as bottom-up grown alloyed germanium-tin ( $\text{Ge}_{1-x}\text{Sn}_x$ ) NWs with  $x = 0.07-0.1$ , diameters of 50-70 nm and lengths of 1 to 3  $\mu\text{m}$ . We are currently working also on the fabrication of alloyed SiGe and SiGeSn NWs with varying content of the different materials.

Next, we will discuss the innovative nanoelectronic devices that we are working on, namely junctionless nanowire transistors (JNTs) and reconfigurable field effect transistors (RFETs). In particular, we are fabricating Si JNTs for sensing application as well as Ge and GeSn JNTs for digital logic. Concerning RFETs, we are currently working on Si RFETs and commencing activities on SiGe and GeSn RFETs, which are expected to outperform the Si RFETs.

Finally, we will briefly present a novel device concept that we recently invented: a specific group IV heterostructure band-to-band tunnel FET (TFET). The fabrication process of this device is scalable and fully CMOS compatible and should allow the achievement of high on-current  $I_{\text{on}}$  together with low off-current  $I_{\text{off}}$ , hence steep subthreshold slope.

## Charging dynamics of self-assembled InAs quantum dots in n-GaAs Schottky diodes

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Self-assembled quantum dots (SAQDs) are used in optical devices like infrared light emitting diodes [1] and lasers [2] and have been studied in relation to flash memory cells [3]. It is therefore important to have a large repertoire of methods available for the preparation and diagnostics of SAQD states and their interaction with the environment. We study the charge transfer dynamics between self-assembled InAs quantum dots embedded in n-GaAs Schottky diodes and the space charge region by Laplace deep level transient spectroscopy (LDLTS). Both filling and emission processes are investigated as a function of temperature and the applied bias voltage [4]. We are able to identify electron tunneling and thermally activated processes and quantitatively model the dynamics within the accessible parameter space. We show that the fundamental problems, which originate from the ill-posed character of the inverse Laplace transform, can be solved by a careful choice of the regularization parameter based on the accurate knowledge of the signal-to-noise ratio.

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## Ultrafast neutralization dynamics of highly charged ions upon impact on 2D materials

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Heavy ions in high charge states carry a large amount of potential energy in addition to their kinetic energy. The potential energy can amount to several 10keV and is released upon neutralization [1]. We recently showed that neutralization of slow highly charged Ar and Xe ions proceeds on a sub-10fs time scale, i.e. during transmission through the very first monolayers of a solid [2]. This feat makes highly charged ions an intriguing tool for efficient modification of 2D materials preventing significant damage to a substrate at the same time. Here we present data on the neutralization dynamics of slow highly charged ions in freestanding single layer graphene and freestanding single layer MoS<sub>2</sub>. Special emphasise is put on charge exchange of the ions, their kinetic energy loss, and the emission of secondary electrons/photons from the interaction process.

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## Ion beam modification of single-layer transition metal dichalcogenides

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Ion irradiation techniques have been extensively used for material modification, post-synthesis engineering and imaging purposes. Although the response of bulk targets to ion irradiation has been studied at length, including simulations, much less is known about the effects of ion bombardment on two-dimensional (2D) materials. 2D transition metal dichalcogenides (TMDs) have shown outstanding physical properties which make them intriguing candidates for various nanoelectronic and optoelectronic applications. We have studied the effects of ion irradiation on freestanding and supported 2D TMDs by using analytical potential molecular dynamics combined with Monte Carlo simulations. We characterized the types and assess the abundance of point defects in our structures as a function of ion energy, mass and incident angle. Furthermore, we studied the irradiation with highly charged ions (HCIs) for fabrication of well-defined pores in MoS<sub>2</sub> monolayer. The simulations indicated a dependence of the pore size on the potential energy of the projectile and suggested an enrichment in molybdenum in the vicinity of the pore edges. These findings help to understand the fundamental physical mechanisms underlying ion irradiation of low-dimensional materials and finding optimum parameters for defect engineering of 2D TMDs with optimized properties.

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## Enhancing of catalytic activity of MoS<sub>2</sub> single layers through spontaneous oxidation under ambient conditions

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The chemical inertness of the defect-free basal plane confers environmental stability to MoS<sub>2</sub> single layers, but it also limits their chemical versatility and catalytic activity. The stability of pristine MoS<sub>2</sub> basal plane against oxidation under ambient conditions is a widely accepted assumption however, we found [1] that oxygen gradually incorporates into the basal plane of 2D MoS<sub>2</sub> crystals through a substitutional oxidation reaction, by replacing individual sulfur atoms, while fully preserving the original crystal lattice during ambient exposure. The scanning tunneling microscopy measurements and DFT calculations reveal a slow oxygen-substitution reaction, during which individual sulfur atoms are replaced one by one by oxygen, giving rise to solid-solution-type 2D MoS<sub>2-x</sub>O<sub>x</sub> crystals. Oxygen substitution sites present all over the basal plane act as single-atom reaction centers, substantially increasing the catalytic activity of the entire MoS<sub>2</sub> basal plane for the electrochemical H<sub>2</sub> evolution reaction. The observed oxidation process enables the chemical modification of single atomic sites of 2D crystals opening new routes towards their efficient defect engineering. This work was supported by the Russian Scientific Foundation (project no. 18-73-10135).

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## Point defects in hexagonal Boron Nitride

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Boron nitride is a promising candidate as a dielectric layer in 2D-material based devices [1]. Bulk hexagonal boron nitride (hBN) is isostructural to graphite, forming a layered honeycomb structure where boron and nitrogen atoms are held together by strong  $sp^2$  bonds, giving hBN excellent mechanical strength and chemical stability [2,3]. Likewise, single layer hBN is also isostructural with graphene. Unlike graphene, however, single layer hBN is an insulator with a nonzero band gap between 5 and 6 eV [4].

In devices, semiconductor function is affected by the presence of intrinsic defects. For example, it is known that oxygen vacancies in semiconducting oxides ( $SiO_2$ ,  $HfO_2$ ) are linked to the filament formation process in resistive RAM devices [5,6]. Studies [7] have shown boron vacancies to be related to the analogous breakdown process in multilayer hBN.

Here we present the results of our investigation into hBN and a collection of its intrinsic defects. Using density functional theory (DFT), we analyse a range of defects in hBN, including boron and nitrogen vacancies, interstitials and Stone-Wells defects. We present the charge transition levels (CTLs), the ground state spin configuration, and the formation energies of the defects.

We use the CP2K software package [8] to implement DFT. This uses a Gaussian type atomic centred basis set and calculates electronic structure in the gamma point. We use a hybrid-DFT functional to calculate exchange and correlation energies. The calculations use  $6 \times 6 \times 4$  supercells in periodic boundary conditions. This particular cell expansion was used to give an effective K-point spacing which would sample the HOMO and LUMO states [9].

The CTLs of the intrinsic defects are calculated and, by alignment with typical electrode workfunctions, it is found that a number of intrinsic defects can be charged during device function. Divacancies are found to have positive binding energy. In particular, the formation of a "molecular bridge" in inter-layer divacancies increases their stability. For example, in the lowest energy configuration of an interlayer boron divacancy, two N atoms form a N-N bridge across the layers. This greatly deforms the surrounding structure and reduces the energy required to form a boron vacancy-interstitial pair. The structure and dynamics of such defects may play a significant role in the breakdown of hBN in nanoelectronic devices.

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## On-surface assembly and reaction of molecular nanostructures: from metals to insulating surfaces

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The interest in molecular nanostructures on surfaces emerges from their prospective applications in nanoscale electronics, solar cells, energy storage devices, and other fields. Non-covalent intermolecular interactions in molecular self-assemblies facilitate the formation of long-range ordered patterns by usage of molecular recognition. In contrast, the stability and intermolecular charge transport are improved in covalent molecular networks fabricated by on-surface reactions, however, at the expense of structural control owing to the irreversible nature of the newly formed covalent bonds.

In my presentation, I will focus on recent high-resolution scanning probe microscopy experiments in combination with density-functional theory about the bottom-up fabrication and electronic properties of atomically precise one- and two-dimensional molecular nanostructures on metals.[1-4] Thereby, the effect of the flexibility, the symmetry, and chirality of the precursor molecules on the structure formation of covalently-linked 2D networks will be discussed.[1-3] I will present how the band gap with the extension of the  $\pi$ -system changes [1] and the observation of delocalized electronic states in surface-supported organometallic networks.[2]

A major challenge in realizing molecular electronic devices is to mechanically stabilize and electrically decouple molecules at and from a surface without losing the control on the structure formation. The electronic decoupling of molecules on insulating surfaces results in a weaker and unspecific molecule-surface interaction, such that molecular assemblies often suffer from diffusion and the assembly of disordered aggregates. Hence, I will conclude with a comparison on the structure formation of molecular self-assemblies on bulk insulator and metal surfaces.

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## Covalent and Non-Covalent Interactions in Molecular Systems

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This talk will concern the development of efficient, yet potentially very accurate, models to describe covalent and non-covalent (van der Waals) interactions in molecular systems. For chemical bonds, we use symmetrized force-based machine learning techniques that allow to achieve the "gold standard" quantum-chemical accuracy in the description of potential-energy surfaces of small and mid-sized molecules. For non-covalent interactions, we have developed coarse-grained quantum-mechanical models for interatomic potentials based on coupled harmonic oscillators. The accuracy, efficiency, and insight that can be obtained from both approaches will be demonstrated and future directions for integrating these models into next-generation quantum force fields for complex molecular systems will be discussed. All our developments are firmly motivated by challenging experimental observations, and we make connections to experiments throughout the talk.

## Kinetic control in molecular self-assembly on an insulating surface

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When molecules are deposited on a crystal surface, it is often expected that they form the thermodynamically most stable structure. However, recent investigations demonstrated that simple benzoic acid molecules deposited on the insulating calcite (10.4) surface upon increase of temperature undergo a series of structural transitions from clusters to an ordered striped network, followed by an ordered dense network, and finally a disordered structure. Here, we combine high-resolution dynamic atomic force microscopy (AFM) and density-functional theory (DFT) to provide a comprehensive analysis of the fundamental principles driving a specific sequence of molecular transitions on insulating calcite. In particular, we elucidate the transition rates of relevant atomistic processes, rationalizing the formation/dissolution of all observed networks. A key finding to understand the observed structural transitions is the system initial state immediately after the deposition, which consists mostly of dimers. Moreover, we argue that the observed sequence of self-assembled structures is entirely controlled by the kinetics of the system, as the smallest energy barriers rather than the thermodynamic stability dictate the specific structural path taken. Finally, we discover a network-assisted dimer dissociation that catalyzes the growth of the dense network. This atomistic insight into the kinetics of on-surface transitions is essential for a detailed understanding of the formation of the observed network sequence (see Figure). Our study, thus, emphasizes the importance of a kinetic control as a promising strategy for achieving tailored molecular architectures on insulator surfaces.

# Posters

Carla Bittencourt

Nanoscale NEXAFS as a search tool for investigating bonding directionality in TiO<sub>2</sub>-B

Magnar Bjorgve

Periodic systems in MRCHEM

Davor Capeta

Dark field optical microscopy of MoS<sub>2</sub> growth and cracking.

Karel Carva

Epitaxial vs. bulk antiferromagnet CuMnAs, the role of defects

Iliia Chepkasov

Atomic structure and electronic properties of few-atom sodium and potassium layers between two graphene sheets

Alexandru Ionut Chirita Mihaila

Influence of temperature on the displacement threshold energy in graphene

Anna Maria Cucolo

Clusters of Vortices induced by magnetic stripe topology in S/F hybrids

Odkhuu Dorj

Towards 2D Nanomaterials Design and Manipulation

Ahmad Echresh

Ion beam implanted Germanium nanowires fabricated by using electron beam lithography

Sadegh Ghaderzadeh

Channeling effects in gold nanoclusters under He ion irradiation: a molecular dynamics study

Arsalan Hashemi

Efficient method for simulating Raman spectra in large supercells and application to transition metal dichalcogenide alloys

Rina Ibragimova

Theoretical study of two-dimensional Ti<sub>2</sub>C and Ti<sub>3</sub>C<sub>2</sub> functionalization process

Heena Inani

Substituting silicon in graphene and carbon nanotubes through intermittent vacancies

Stig Rune Jensen

Pushing the limit of reproducibility in molecular and solid-state calculations

Thomas Joseph

Non-stoichiometric phases of 2D transition metal dichalcogenides: a computational study

Marc Jäger

Efficiently Computing Adsorption Energy Distributions on Nanoclusters

Zhennan Kou

An empirical potential study of first-order Raman scattering in defective MoS<sub>2</sub>

Marko Kralj

Atomic-scale defects and electronic properties of synthesized MoS<sub>2</sub> monolayer

Ondrej Krejci

Complex Probe Particle Model Simulations Supporting nc-AFM Experiments

Silvan Kretschmer

Exciting! - Damage mechanisms in two-dimensional MoS<sub>2</sub>

Dominik Legut

Two dimensional protective films for lithium and sodium metal anodes

Ursula Ludacka

Measuring and Controlling Out-of-Plane Shape of Free-Standing Two- Dimensional Materials

Konstantin Mukhin

Pelletized IBR-2 reactor cold neutron source for nanoscale science experiments

Janne Nevalaita

Free-standing two-dimensional metals: from infinite sheets to edges and vacancies

Marin Petrović

Interface engineering within the lateral heterostructures of hexagonal boron nitride and graphene

Igor Poltavskji

Quantum Tunneling of Thermal Protons Through Pristine Graphene

Clémence Queffélec

Plasmonic nanoparticles for sensor devices

Yashasvi Singh Ranawat

Descriptor design and selection for hydrogen evolution reaction

Zamaan Raza

Linear scaling first principles constant pressure molecular dynamics in Conquest

Janine Schwestka

Ion-induced electron emission from 2D materials

Dmitry Terentyev

Modelling of hydrogen retention in tungsten based on ab initio calculations

Stepan Tsirkin

Higher-Order Topological Defect States in Insulators

Fedor Urtev

Deep learning in aid to high resolution AFM experiments

Li Wenjiang

In-situ growth of MoS<sub>2</sub> Nanoparticles on Reduced Graphene Oxide Aerogels for Efficient HER Electro-catalysis

Georg Zagler

Growth and Characterization Thin Films on Graphene in Ultra High Vacuum



## Nanoscale NEXAFS as a search tool for investigating bonding directionality in TiO<sub>2</sub>-B

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TiO<sub>2</sub> nanostructures exist in different crystallographic phases including brookite, anatase, rutile, and TiO<sub>2</sub>-B (bronze). Among these, due to its open channel-like crystal structure which can enhance ion mobility, the TiO<sub>2</sub>-B phase has been reported as an optimal anode material for lithium ion batteries, particularly in the form of nanowires [1]. In view of device applications, where different phases may coexist and TiO<sub>2</sub>-B particles may transform to the thermodynamically stable anatase phase, it is important to identify and understand the structural and electronic differences between these two phases. Here we have studied the electronic structure of TiO<sub>2</sub> nanoribbons in TiO<sub>2</sub>-B and anatase phases using polarization dependent near-edge X-ray absorption fine structure spectroscopy (NEXAFS) in the transmission X-ray microscope (TXM) and density functional theory (DFT) [2,3]. NEXAFS at both the O K-edge and the Ti L-edge is very sensitive to the local bonding environment in TiO<sub>2</sub>-based materials and thus provides diagnostic information about the crystal structures and oxidation states. We report the observation of strong linear dichroism in the O K-edge spectra of single TiO<sub>2</sub>-B nanoribbons. Using DFT calculations we show that the dichroism is a consequence of the directional Ti-O bonding in the monoclinic crystal structure.

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## Periodic systems in MRCHEM

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The MRCHEM code is a numerical real-space code for molecular electronic structure calculations within the self-consistent field (SCF) approximation of quantum chemistry (Hartree-Fock and Density Functional Theory), using the Multiwavelets (MWs) basis.

MWs is constructed to have good mathematical properties (convergence, error control, completeness, sparsity) The first application in quantum chemistry appeared in 2004 by Harrison and coworkers [1]. Following their pioneering work our group has developed an independent MW code [2] for Hartree-Fock and DFT, which is able to handle closed and open shell systems, and has recently been applied to two large and precise, benchmark studies on electronic energies [3] (211 molecules with guaranteed micro-Hartree precision with respect to the basis set limit) and magnetizabilities and shielding constants [4] (28 molecules, 0.01 parts per million precision, with respect to the basis set limit).

The goal of this project is to achieve similar accuracy for the modeling of materials and their properties. In this poster we show our progress using MWs on periodic systems. The examples will contain simple, proof of concept SCFs, displaying the precision of solutions to periodic systems, using our new python interface VAMPyR.

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## Dark field optical microscopy of MoS<sub>2</sub> growth and cracking.

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Dark field optical microscopy is powerful tool for visualizing small objects, often much smaller than the wavelength. It is based on illuminating substrates in such a way that only scattered light is collected by imaging optics. The method has been long used in semiconductor industry for detecting contamination and scratches on wafers. It is also used for nanoparticle tracking and counting. We show that this method can be used to visualize features in MoS<sub>2</sub> flakes and layers, including those that are not visible in reflected light, such as grain boundaries, cracks and wrinkles. Basic theory of such scattering, including angular and wavelength dependence is presented. We built miniature CVD system that permits lateral illumination of substrates during growth. This enables observation of the growth process both in dark field or bright field using long working distance microscope objective. Evolution of flakes and defects, from nucleation through growth to merging of flakes is directly observed. We also show that strained MoS<sub>2</sub>, produced by rapid cooling after growth, is relatively stable until exposure to ambient conditions. Process of cracking is observed in real time and resulting structures are characterized using usual methods.

## Epitaxial vs. bulk antiferromagnet CuMnAs, the role of defects

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The antiferromagnetic semimetal CuMnAs has recently attracted attention of physicists due to its potential in spintronics. A controlled rotation of magnetic moments' orientation by means of an applied electrical field has been demonstrated in tetragonal CuMnAs, employing spin-orbit torques [1]. This effect allows for creation of a unique non-volatile memory device faster than flash memory and robust against magnetic field. Furthermore, it can be used to construct micron-size bit cells acting as a multi-level memory-counter [2] with potential applications in nanoelectronics. However, bulk CuMnAs natively crystallizes in the orthorhombic phase, which has different interesting properties. Tetragonal CuMnAs phase has been achieved in epitaxially deposited samples or by inserting lattice defects linked to non-stoichiometry in CuMnAs [3]. Electronic, magnetic, and transport properties of the antiferromagnetic (AFM) CuMnAs alloy with both tetragonal and orthorhombic structure are studied here from first principles using the total energy calculations [4]. We have estimated the stability of different phases and calculate formation energies of possible defects in the alloy.  $Mn_{Cu}$  and  $Cu_{Mn}$  antisites and vacancies on Mn or Cu sublattices were identified as most probable defects in CuMnAs. We have found that the interactions of the growing thin film with the substrate and with vacuum are important for the phase stability of real samples prepared as a thin film on the appropriate substrate. We estimated also the in-plane resistivity of CuMnAs with defects of low formation energies. Our numerical simulations fitted experiment very well if we assumed concentrations 3.5-5%  $Mn_{Cu}$  antisites in the samples, much larger concentrations would be needed for  $Cu_{Mn}$  antisites or Mn-vacancies [4]. Finally, we have determined the exchange interactions and estimate the Néel temperature of the ideal and disordered AFM-CuMnAs alloy using the Monte Carlo approach. A good agreement of the calculated resistivity and Néel temperature with experimental data makes it possible to estimate the structure and composition of real CuMnAs samples.

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## Atomic structure and electronic properties of few-atom sodium and potassium layers between two graphene sheets

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Recent investigations of lithiation and delithiation of bilayer graphene showed that formation of a multilayer close-packed Li phase between graphene sheets is possible [1]. The formation of such a close-packed multilayer phase of lithium allows to increase the areal Li storage capacity (160 nAh/cm<sup>2</sup> for three atomic layers of Li and 28 nAh/cm<sup>2</sup> for the C<sub>6</sub>LiC<sub>6</sub> phase). Sodium-ion batteries and potassium-ion batteries (PIBs) have also rapidly developed. However, the formation of multilayer phases of sodium and potassium between the graphene layer has not previously been investigated. In this paper, using the density functional theory, we study the intercalation of sodium and potassium atoms into bilayer graphene with the main focus on the redistribution of electron density for different numbers of sodium and potassium layers. The reported study was funded by Ministry of education and science of Russian Federation and German Academic Exchange Service (DAAD) according to the research project No 57391663.

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## Influence of temperature on the displacement threshold energy in graphene

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The atomic structure of nanomaterials is often studied using transmission electron microscopy. In addition to image formation, the energetic electrons may also cause damage while impinging on the sample. In a good conductor such as graphene the damage is limited to the knock-on process caused by elastic electron-nucleus collisions. This process is determined by the kinetic energy an atom needs to be sputtered, ie, its displacement threshold energy. This is typically assumed to have a fixed value for all electron impacts on equivalent atoms within a crystal. Here we show using density functional tight-binding simulations that the displacement threshold energy is affected by the thermal perturbation of the atoms from their equilibrium positions. We show that this can be accounted for in the estimation of the displacement cross section by replacing the constant threshold value with a distribution. The improved model better describes previous precision measurements of graphene knock-on damage, and should be considered also for other low-dimensional materials.

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## Clusters of Vortices induced by magnetic stripe topology in S/F hybrids

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Many of the potential applications of superconductors in electronic devices demand high current densities with minimal losses, requiring a mandatory pinning of vortices. In the last decade several studies have focused on the influence of different types of pinning centers on the dynamics of superconducting vortices in type-II superconductors [1-2]. Among them, magnetic pinning in magnetically coupled superconductor/ferromagnet (S/F) heterostructures, appears to be stronger than other mechanisms. Particularly, an enhanced pinning has been reported due to vortex coupling with ordered magnetic structures, such as stripes and dots [3-4]. Nevertheless, unconventional vortex configurations such as vortex chains, vortex clusters as well as multi-vortex and giant vortex phases can also be induced by a strong magnetic or geometric confinement potential [5-6]. In this work, we used low-temperature MFM to investigate S/F heterostructures composed of Py as the magnetic material and Nb as the superconductor, with several Py and Nb thickness, separated by a thin SiO<sub>2</sub> insulating layer to prohibit proximity effects. A thick Py film presents peculiar arrangement of magnetic domains, made by stripes with canted magnetization vectors, mainly oriented along the film plane, but with small alternating up-and-down out-of-plane components. Moreover, its Curie temperature  $T_C$  is much greater than the superconducting critical temperature  $T_S$ , ensuring a field cooling of Nb in a spatially nonuniform magnetic field, giving place to vortices with opposite polarities, namely Vortices and Antivortices (V and AV). We investigated the conditions for nucleation of spontaneous V-AV structures as a function of thickness of superconducting films as well as magnetic domain width. We compared our results with those of existing theoretical models and provided an estimate of the threshold of the local out-of-plane component of the magnetization for different Py film thickness. In this sense, the MFM imaging of spontaneous V-AV in Nb/Py bilayers, for different Nb and Py thickness, is also proposed as an indirect but quantitative method to estimate the out-of-plane magnetization value of our F layers [7-8]. Moreover, the periodic out-of-plane stray field coming out from Py surface plays the role of magnetic confinement potential for vortices, forcing those to align in chains along the domains. When in presence of intrinsic topological defects of the magnetic template, called

bifurcations, we found a peculiar distribution of superconducting vortices. In such cases, we demonstrated that a bifurcation can naturally lead to unusual vortex distribution, and eventually to the formation of vortex clusters, without any need of invasively engineering the shape of the sample via lithography or self-assembly. MFM measurements clearly show that a bifurcation, where two magnetic stripe domains converge and coalesce in a single one, leads to a local enhancement of the out-of-plane stray field. As imaged by MFM, this enhancement induces vortex clusters. We infer that such a phenomenon can be also explained by taking into account the role of the bifurcation magnetic topology. Indeed, while each vortex inside an infinite chain would feel the same net repulsive force, which leads to a constant intervortex distance, an unbalanced force is felt by vortices close to magnetic channel interruptions (stripe endpoint or bifurcation core). For instance, the vortex at the stripe endpoint feels a long-range repulsive interaction due to the semi-infinite vortex chain on one side, while on the other side only the Lorentz force would keep it away from the domain wall. In such a case a reduction of the inter-vortex distance close to the magnetic stripe endpoint is expected. The bifurcation topology in directly affects the vortex distribution at the nearest neighbour domains as well. Indeed, our experimental results show that Hexagonal vortex lattice is achieved at the matching field wherever the stripes are straight and regular, as expected. On the other hand, around the dislocations the inter-vortex distance is affected by the stripe curvature, leading to a modulation of the vortex-vortex spacing.

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## Ion beam implanted Germanium nanowires fabricated by using electron beam lithography

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Germanium (Ge) is a promising high mobility channel material for future nano-electronic devices with a lower effective charge carrier mass than Silicon (Si), which results in a higher electron ( $\times 2$ ) and hole ( $\times 4$ ) mobility. Materials with high carrier mobility can enable increased integrated circuit functionality or reduced power consumption. Hence, Ge based nanoelectronic devices could offer improved performance at reduced power consumption compared to Si electronics. Doping or the introduction of impurity atoms allows the tuning of the electrical properties of the semiconductor material. Ion beam implantation is an industrial standard for semiconductor's doping as it can incorporate single ion species with a single energy in a highly controlled fashion. The destructive nature of ion implantation doping due to the deposited energy and resultant cascade of recoils within the nanowire volume requires a crystal recovery step such as an annealing process. In this work, Ge nanowires were first fabricated using electron beam lithography (EBL) and inductively coupled plasma (ICP) etching. Then ion beam implantation was used to introduce phosphorous (P) dopant atoms into Ge nanowires. Afterwards, flash lamp annealing (FLA) was applied to recover the crystal structure of Ge nanowires and activate the dopant atoms. Micro-Raman spectroscopy spectra showed that, by increasing the fluency of ion implantation, the optical phonon mode of Ge peak was broadened asymmetrically. This is related to the Fano effect and shows that dopant atoms are placed in substitutional positions and are electrically activated. Moreover, we are designing three- and four-probe Hall Effect measurement configurations for single Ge nanowires to determine their mobility and carrier concentrations.

## Channeling effects in gold nanoclusters under He ion irradiation: a molecular dynamics study

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Ion channeling is a well-known effect in ion irradiation processes, which is a result of ion moving between the rows of atoms. It drastically affects the ion distribution, ion energy-loss and consequently the damage production in the target. Therefore one could derive the ion-channeling pattern out of the energy-loss behavior of ion-target interaction. Ion channeling effect is studied for a few pure element crystals and also for some compounds in a systematic way[1]. In this work, we focus on nano-structures which are of major importance, due to their high surface-to-volume ratio. Our results, for different gold cluster sizes, show that ion-channeling occurs not only in the principal low-index, but also in other directions in between. The strengths of different channels are specified, and their correlations with sputtering-yield and damage production is discussed.

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## Efficient method for simulating Raman spectra in large supercells and application to transition metal dichalcogenide alloys

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Raman spectrum can be simulated using first-principles methods, but due to the computational cost, it is usually limited only to fairly small unit cells, which then excludes carrying out these simulations for alloys. Here, we develop an efficient method for simulating Raman spectra of alloys, benchmark it against full density-functional theory calculations, and apply it for few different alloys of transition metal dichalcogenides. The method is based on the projection of the vibrational modes of the supercell to those of the primitive cell, for which full first principles Raman calculations are performed. This approach is not limited to 2D materials and should be applicable in many different material systems. Furthermore, mass approximation is adopted to efficiently evaluate the supercell vibrational modes, but is limited to chemically and structurally similar atomic substitutions. To benchmark our method we first apply it for the  $\text{MoxW(1-x)S}_2$  in the H-phase, where several experimental reports are available for comparison. Next, we consider  $\text{MoxW(1-x)Te}_2$  in the T'-phase, which has been proposed to be a 2D topological insulator, but where experimental results for the monolayer alloy are still missing. Finally, we search for characteristic Raman signatures for impurities in  $\text{MoS}_2$  in the dilute concentrations.

## Theoretical study of two-dimensional $Ti_2C$ and $Ti_3C_2$ functionalization process

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MXene phases are a new rapidly developing class of two-dimensional materials with suitable electronic, optical and mechanical properties for different applications [1]-[3]. These phases consist of transition metals such as Ti, Sc, Zr, Hf, V, Nb, Ta, Cr, Mo and carbon or nitrogen atoms, and can be produced through the etching of layered MAX phases. During the etching process, it is possible to terminate the surface by O, OH, and F functional groups in order to modify materials properties [4][6]. In this work, we accurately describe the surface distribution of functional groups and its interaction with titanium-based two-dimensional carbides in the solution through the use of different approaches. The free Gibbs energies of formation for the distinctly terminated surfaces have been studied by combining DFT, phonon calculations and implicit solvation model. Our results indicate the formation of O, OH and F mixture, which coincides with experimental data [ 1]. Furthermore, DFT together with cluster expansion (CE), and Monte Carlo methods are employed to investigate the distribution of the functional groups on the surface. The proposed computational approach allows us to deeper understand a functionalization mechanism and introduce the range of experimental conditions for further tuning the MXenes properties.

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## Substituting silicon in graphene and carbon nanotubes through intermittent vacancies

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The band structure of single-walled carbon nanotubes (SWCNTs) is entirely determined by the cutting direction and the dimensions of the graphene slab the tubule is constructed from. Synthesizing nanotubes with a desired configuration has proven immensely difficult and alternative routes to tune the properties are still being sought for. One promising approach is substitutional doping by impurity elements [1]. Here, by simultaneous plasma and laser irradiation of a SWCNTs-graphene van der Waals heterostructure, we incorporate silicon heteroatoms in both materials. The vacancies thus created are primarily healed by thermally diffusing carbon and Si atoms, the latter of which we directly identify in the lattice by using atomic resolution scanning transmission electron microscopy. In SWCNTs, these atoms are found in 3-coordinated, 4-coordinated and not identifiable configurations with recurrence of 61%, 36% and 3%, respectively and thus in good agreement with earlier theoretical predictions for single and double vacancies [2]. These 1D-nanostructures doped with Si heteroatoms may show up as a promising candidate for water splitting, gas sensing and drug delivery applications.

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## Pushing the limit of reproducibility in molecular and solid-state calculations

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There has been much focus in the literature in recent years on the reproducibility of numerical results across different computational platforms[1]. While reproducibility of results is one of the fundamental pillars of science, it cannot always be guaranteed within the computational disciplines, where calculations that in principle should be equivalent sometimes can vary significantly due to either elaborate algorithmic approximations, subtle implementation specific details or even plain bugs in the software.

For molecular calculations we believe that the issue can be put to rest, at least within the non-relativistic single-particle models, as it has been shown that a hard numerical reference can be obtained through all-electron calculations using a multiwavelet basis set[2]. Multiwavelets are both systematic and unbiased, and makes it computationally feasible to reach a numerical precision that is orders of magnitude beyond any of the standard computational methods, which has been demonstrated for a variety of molecular properties.

We will here discuss the mathematical framework which makes this possible, and highlight some of the work we have done in recent years on benchmarking molecular calculations[3,4]. Finally we will show some preliminary results on the extension of our methods to extended systems and solid-state physics.

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## Non-stoichiometric phases of 2D transition metal dichalcogenides: a computational study

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Changing the stoichiometry of a material in a controllable manner is a powerful tool to tailor the structure and the properties of a compound solid. For example, new morphologies, such as inversion domains with the associated mirror twin boundaries [1] can be produced in 2D transition metal dichalcogenides by sputtering chalcogen atoms using electron beam [1]. Moreover, suspended monolayer Mo membranes were recently fabricated from monolayer MoSe<sub>2</sub> sheets via complete sputtering of Se atoms in a scanning transmission electron microscope [2]. Motivated by these results, we performed first-principles calculations to understand the energetics of 2D phases of binary compounds which can be referred to as strongly non-stoichiometric transition-metal dichalcogenides. The 2D phases were assumed to be formed by the formation and aggregation of vacancies in the pristine system. The formation energies of the 2D materials with different stoichiometries are analyzed for a wide range of chemical potentials. The results show that these phases become energetically favourable only when the system is locally charged.

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## Efficiently Computing Adsorption Energy Distributions on Nanoclusters

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Machine learning and automation will drastically reduce computational cost and research labor costs in materials science. Catalysis on nanocluster surfaces is a prime subject where such an approach is beneficial, since after significant advancement in producing nanoparticles with defined composition, size and morphology in the last decade [1, 2], another exploration dimension has opened up where suitable catalysts can be found. Density Functional Theory (DFT) models chemical properties of the nanoclusters important for catalytic activity, such as the adsorption free energy ( $\Delta G_H$ ). However, since the search space is so large, the screening becomes too expensive even with DFT. Machine learning can fill in the gaps so that not every single catalyst configuration needs to be computed by DFT.

We present an automated workflow based on the workflow manager Fireworks which takes care of repetitive tasks and reaches a high level of automation. High-symmetry nanoclusters (icosahedra, octahedra and Wulff-shaped) are constructed before their surface adsorption sites get detected as top, bridge or hollow. Based on the structural descriptor SOAP [3] the adsorption sites are ranked prior to being most distinct from each other. This allows an efficient computation of adsorption energies with the linearly scaling DFT code CP2K in the next step where redundant sites are eliminated. Finally, the adsorption energy distribution of the cluster surfaces is predicted via kernel ridge regression. The workflow automatically stops as soon as a sufficient accuracy is achieved.

A small dataset of bimetallic transition metal nanoclusters is showcased containing the elements Fe, Co, Ni, Cu, Mo and Pt at different compositions. We determined the adsorption energy distributions of 41 nanoclusters and pinpointed regions of metal compositions which are potentially active for the hydrogen evolution reaction.

We intend to make a software package publicly available in the near future which allows several scientists to contribute to a nanocluster database simultaneously.

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## An empirical potential study of first-order Raman scattering in defective $\text{MoS}_2$

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Two-dimensional (2D) materials offer interesting and unique properties for devices. The existence of structural defects can play either detrimental or beneficial roles, depending on the targeted application. Raman spectroscopy is known as an important and versatile tool for the characterization and the control of defects. A wide range of scales are covered through empirical potential approach, to determine Raman activity at low concentrations, and to specify the role of higher defect concentration and defect disorder respectively. In order to extract relevant modes out of performed calculations, and to yield approximated peak shape, the band unfolding scheme is used. As a result, we find out i) How the peaks from pristine system evolve upon increasing defect concentration. ii) Are the changes common for all point defects or they depend on the defect. iii) How the defect size affects the results, i.e., the vacancy density vs. defect density in the case where one defect contains more than one vacancies.

## Atomic-scale defects and electronic properties of synthesized MoS<sub>2</sub> monolayer

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Significant scientific and technological interest in two-dimensional (2D) materials is closely related to the fact that today's microelectronic devices are based on 2D architectures. Special attention is dedicated to intrinsically semiconducting 2D materials, where molybdenum disulphide (MoS<sub>2</sub>) monolayer is a prominent member of the transition metal dichalcogenide family.

MoS<sub>2</sub> researched in this work were synthesized on a SiO<sub>2</sub>/Si wafer and transferred to Ir(111) for nano-scale characterization. The established transfer procedure is applicable to a diversity of substrates, thus opening a way to different applications. Samples were extensively characterized during every step of the transfer process, and MoS<sub>2</sub> on the final substrate examined down to the atomic level by scanning tunneling microscopy (STM). Conducted procedures yielded high quality monolayer MoS<sub>2</sub> of millimeter-scale size with an average defect density in the same range as samples obtained by exfoliation from the natural MoS<sub>2</sub> [1]. By combined use of STM imaging and density functional theory (DFT) calculations we identified the most recurring point-like defects as S vacancies. The electronic band gap measured by scanning tunneling spectroscopy (STS) revealed n-doping of the samples and lateral nano-scale variations of the band gap. From the difference of the electronic band gap measured by STS of 2.1 eV and the optical band gap measured by photoluminescence (PL) of 1.9 eV, an estimated exciton binding energy of 0.2 eV is obtained. Comparison of experimental results and simulations considering freestanding and epitaxial MoS<sub>2</sub> on Ir(111) leads to the conclusion that the investigated samples on Ir(111) are quasi-freestanding or weakly coupled to the substrate, based on the observation of the semiconducting band gap, nano-scale rippling of flakes and weak binding of flake edges [2].

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[2] I. Dela Marion et al., *Nanotechnology* **29**, 305703 (2018).

## Complex Probe Particle Model Simulations Supporting nc-AFM Experiments

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I will present results concerning simulations of scanning probe microscopy experiments. Main focus will be on simulations of systems studied experimentally with a CO-tip AFM/STM. First of them is a hexagonal boron-nitride grown on Ir(111) surface. In the AFM experiments acquired with a CO-tip an unexpected contrast was observed. Simulations using complex electrostatics [1] of the tip helped us to understand the origin of the contrast [2]. The other systems are non-planar molecules adsorbed on Cu(111) and Au(111) surfaces. Simulations employing more realistic description of the CO tip [3], than the standard probe particle model [4,5], were found to be important for better agreement of the theoretical simulations to experimental data on 3D molecules [6]. Together with description of the experiment and DFT calculations of the systems, the presentation will also contain details about development of the probe particle AFM model [4,5].

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[2] F. Schulz, J. Ritala, O. Krejci, A. S. Seitsonen, A. Paavo, A. S. Foster and P. Liljeroth, *ACS Nano* **12** (6), pp 5274-5283 (2018).

[3] M. Di Giovannantonio, J. I. Urgel, U. Beser, A. V. Yakutovich, J. Wilhelm, C. A. Pignedoli, P. Ruffieux, A. Narita, K. Mllen, and R. Fasel, *J. Am. Chem. Soc.* **140**, 3532 (2018).

[4] P. Hapala, G. Kichin, C. Wagner, F. S. Tautz, R. Temirov, and P. Jelinek, *Phys. Rev. B* **90**, 085421 (2014).

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- [6] S. Kawai, O. Krejci, A. S. Foster, R. Pawlak, F. Xu, L. Peng, A. Orita and E. Meyer, *ACS Nano* **12** (8), pp 8791-8797 (2018).

## Exciting! - Damage mechanisms in two-dimensional MoS<sub>2</sub>

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As the influence of defects on material properties heavily depends on the dimensionality, understanding defect production mechanisms in detail plays a major role for two-dimensional (2D) materials. The defect production under irradiation e.g. in the transmission electron microscope (TEM) can be subdivided into three mechanisms, namely knock-on damage, ionization damage and chemical etching. Surprisingly, as shown for transition metal dichalcogenides, in TEM defects are produced far below the knock-on threshold [1]. Here we investigate the combination of excitation and knock-on damage mechanisms in two-dimensional MoS<sub>2</sub> under electron beam by using advanced first-principles simulation techniques.

[1] Y.Lin, T.Björkman, H.Komsa et. al. , *Nature Communications* 6, 6736 (2015).

## Two dimensional protective films for lithium and sodium metal anodes

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Rechargeable batteries based on lithium or sodium metal anodes have been attracting increasing attention due to their high capacity and energy density, but exhibit drawbacks, such as low Coulombic efficiency and dendrites growth. Layered materials have been used experimentally as protective films (PFs) to address these issues. Here we use first-principles calculations to determine the properties and feasibility of various 2D layered PFs, including the defect pattern, crystalline structure, bond length, and metal proximity effect, Li<sup>+</sup> (Na<sup>+</sup>) ion diffusion and mechanical stability. It is found that the introduction of defect, the increase in bond length, and the proximity effect by metal can accelerate the transfer of Li<sup>+</sup> (Na<sup>+</sup>) ion and improve the ionic conductivity, but all of them make negative influences on the stiffness of materials.

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## Measuring and Controlling Out-of-Plane Shape of Free-Standing Two- Dimensional Materials

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In this work, we show through transmission electron microscopy (TEM) and atomistic simulations that the non-flatness of free-standing graphene, hBN, and MoS<sub>2</sub>, as well as their heterostructures varies depending on the material. Out of all studied materials, graphene is the least flat, followed by hBN and finally MoS<sub>2</sub>. For the heterostructures, the overall shape is determined to a large extent by the stiffer of the two materials.

In addition to measuring the out-of-plane shape, we can also control it in situ in one direction using a stretching holder. For these experiments, we glued the samples, transferred onto gold TEM grids with a perforated amorphous carbon film, onto the holder and applied mechanical strain with small incremental steps to avoid breaking the film during the experiment. The deviation of circular symmetry of the diffraction pattern and the shape of the individual diffraction spots give us insight on the strain in the material and its out-of-plane shape, respectively.

Our results show that this simple method can be used to completely flatten the 2D materials in the direction of the applied force. At this point, the material exhibits an aligned set of one-dimensional corrugations. After the structure has been flattened, continuous mechanical deformation leads to a measurable strain in the structure.

## Pelletized IBR-2 reactor cold neutron source for nanoscale science experiments

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IBR-2 is a pulse reactor for neutron research. Flux of thermal neutron is about  $10^{13}$  n/cm<sup>2</sup>·sec. Cold neutrons with wavelengths over 4 Å emitted by high-current neutron sources have been employed in physical research since the 1980s. Cold neutrons scattering in big moleculars and atom's groups and see diffraction peaks in a high wavelength region. Like a result using the cold moderator get a better resolution on spectrometers and diffractometers. At the same time an experiment time can be less by the moving a neutron peak to big neutron's wavelength region. The cold-neutron flux is enhanced by using neutron moderators cooled to low temperatures. In these, neutrons are retarded when passing through different substances such as water, heavy water, ice, paraffin, beryllium, liquid hydrogen, liquid and solid methane, and various hydrocarbons. A neutron gradually loses its kinetic energy through multiple collisions with the nuclei of the moderator material. In a modernization of IBR-2 reactor in 2006 was project of creation a cold neutron source. The source included three combine moderators around a reactor core. Moderators have a similar principle of work but different configuration of head part. The combine moderator is a different technical construction witch consist of a cold chamber (20K - 100K) for getting neutrons with long wavelengths and warm chamber (in some of it a water pre-moderator) for thermal neutrons. The substance for slowing neutrons on IBR-2 cold source was choose a mezeilene on solid phase and beads form. In the presentation will be shown steps of creation the combine moderator of the "central" direction (CM201) of IBR-2 reactor on mezeilene pellets. Calculations and choosing a different various of configuration CM 201 moderator. Technical equipment for the moderator system. Experiment on full scale model of moderator CM201. Will be shown a dependent a neutron spectrum from temperature of moderator. The results of the test exploitation combine moderator (CM202) with some examples of experiments on a High Resolution Fourier Diffractometer (HRFD), a multiresearch diffractometer DN-6, a strain/stress diffractometer EPSILON-MDS and an Inverted geometry time-of-flight spectrometer.



## Free-standing two-dimensional metals: from infinite sheets to edges and vacancies

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Experimental discovery of atomically thin iron patches inside graphene nanopores [1] added a new member to the expanding family of two-dimensional (2D) materials by sparking computational research of free-standing metal atom monolayers. Due to the potential in catalytic, magnetic and optical properties of these 2D metals, they have numerous possible applications [2] and, contrary to common covalently bonded 2D systems, the flexible metallic bonding can even form a 2D liquid in simulations [3]. Using density functional theory (DFT), we have systematically studied 45 metal monolayers in three crystal structures and found that their cohesive energies, equilibrium distances, and bulk moduli are broadly inherited from the corresponding 3D structures [4]. Based on calculated elastic constants, the square lattice appears unstable against in-plane deformations for most metals. To address more realistic systems, we have also calculated the edge and vacancy formation energies [5]. The edge energy behaves analogously to surface energy, decreasing with increasing Wigner-Seitz radius of the metal and 2D vacancy formation energy is close to the 3D one. These trends provide useful insights when moving towards reality with elemental 2D metals.

[1] J. Zhao, Q. Deng, *et al.*, *Science* **343**, 1228 (2014).

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## Interface engineering within the lateral heterostructures of hexagonal boron nitride and graphene

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Integration of 2D materials into heterostructures is a very important step towards utilization of atomically-thin systems in future technologies. In order to tailor the properties of the heterostructures as desired, it is crucial to understand the details of their synthesis and fabrication, including possible routes for controlling the properties of the interface between individual 2D materials that constitute the heterostructures. By using low-energy electron microscopy (LEEM), photoemission electron microscopy (PEEM), and selected-area low-energy electron diffraction ( $\mu$ -LEED), we study lateral heterostructures of hexagonal boron nitride (hBN) and graphene on Ir(111) [1]. The heterostructures are synthesized by sequential chemical vapor deposition from borazine and ethylene, and this process is tracked in situ in ultrahigh vacuum with LEEM. It is found that, besides hBN (an insulator) and graphene (a conductor), a 2D alloy consisting of hexagonally arranged B, C and N atoms (hBCN, a semiconductor) is formed on the iridium surface at the interface between hBN and graphene. hBCN alloy originates from the intermixing of borazine and ethylene fragments, and therefore its stoichiometry and spatial extension can be tuned by modifying the parameters of the synthesis (most notably temperature and precursor dosage), which also allows for the production of material with nanoscale-modulated properties. Stoichiometry, i.e. relative carbon concentration determines the size of hBNC direct bandgap [2], and the potential to arbitrarily set the gap size is of high interest for, e.g., photovoltaic or lasing applications of 2D materials.

[1] M. Petrović et al., *Appl. Surf. Sci.* **455**, 1086 (2018).

[2] M. Zhang et al., *Nanoscale* **7**, 12023 (2015).

## Quantum Tunneling of Thermal Protons Through Pristine Graphene

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Atomistic modeling of nanoscale materials from first principles often requires involving quantum mechanics for an accurate description of the nuclear dynamics. For instance, the experimentally observed appreciable permeability of graphene and hexagonal boron nitride to thermal protons [S. Hu *et al.*, *Nature* 516, 227 (2014); M. Lozada-Hidalgo *et al.*, *Science* 351, 68 (2016).] remains unexplained by density-functional electronic structure calculations, which yield Arrhenius activation energies that exceed by  $\sim 1.0$  eV those found in experiments. We demonstrate that the thermal proton transfer through pristine graphene is driven by nuclear quantum effects, which substantially reduce the value of Arrhenius activation energy by up to 1.0 eV compared to the results of classical simulations. In contrast, the transport of heavier hydrogen isotopes, such as deuterons, at the same conditions is mainly led by classical processes. This qualitative difference in transport mechanisms offers new insights for controlling the ion separation by nanostructured membranes.

## Plasmonic nanoparticles for sensor devices

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Surface enhanced Raman spectroscopy (SERS) is a well-established technique used for the sensing of molecular and ionic species in solution and the vapor phase with extremely low detection limits.[1] Of particular interest to us is the detection of metal ions in aqueous media using a thin-film SERS sensor. Metallic nanoparticles (NPs) have many useful properties, in particular some NPs have unique optical qualities while interacting with light known as surface plasmon resonance (SPR). The platform chosen for the detection of metal ions using the SERS technique was developed previously in our labs for the blue-laser enhanced copper(I) catalyzed Ullmann coupling reaction.[2] The protocol uses the hydrolysis of titanium(IV) isopropoxide in water in the presence of silver nanoparticles to prepare stable core-shell Ag@TiO<sub>2</sub> nanoparticles. Then, the resulting NPs have been functionalized by a 2,2'-bipyridine-based ligand (L) bearing a phosphonic acid tether to ensure an ionic-covalent anchoring onto TiO<sub>2</sub> to form Ag@TiO<sub>2</sub>@L. In the last step, metal ions reacted with Ag@TiO<sub>2</sub>@L to form Ag@TiO<sub>2</sub>@L-M nanocomposites. In Raman spectroscopy, the film of Ag@TiO<sub>2</sub>@L was recorded at 514, 633 and 785 nm with low power of the focused laser. The spectrum was dominated by the vibrational modes of the bipyridine group. The SERS spectrum of Ag@TiO<sub>2</sub>@L-M was recorded for references at the three wavelengths. Finally, to determine the sensitivity of the Ag@TiO<sub>2</sub>@L platform towards ions in aqueous solvent, thin films of Ag@TiO<sub>2</sub>@L were treated with successively dilute concentrations of metal ions (nickel, copper, rhodium, manganese sources) in water and dried under a flow of argon, followed by heating to 60 °C prior to Raman spectroscopic analysis. Signals due to the presence of metal ions were easily observed down to a picomolar concentration. Femtomolar concentrations were also detected however, contamination from the glassware or lab environment cannot be excluded in this case. By tuning the laser wavelength, different spectral features were obtained according to the metal thus future work will be directed towards selective detection of metal ions and recycling of the sensor platform.

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## Descriptor design and selection for hydrogen evolution reaction

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Catalyst design is a crucial aspect of hydrogen evolution reaction (HER). It is aided by rigorous simulations of catalytic action on suitable candidates. However, this is non-trivial due to an infinite search space, and computationally intensive DFT simulations. Here, machine-learning aided approaches can be applied to augment the database of catalysts, and also select the relevant catalyst. Since computers cannot inherently understand the rotational, translational, or permutational invariance of atomic representation, various representations of chemical environment – descriptors – are introduced. The study compares the descriptors: SOAP, an electronic description based on SOAP and local adaptation of MBTR, to outline their applicability in predicting adsorption-energy for HER.

- [1] Marc O. J. Jager, Eiaki V. Morooka, Lauri Himanen, Filippo Federici Canova, Adam Foster, *NPJ Computational Material* **4.1**, 37 (2018).
- [2] Bartok, Albert P., Risi Kondor, and Gabor Csanyi, *Physical Review B* **87.18**, 184115 (2013).
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## Linear scaling first principles constant pressure molecular dynamics in Conquest

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Density functional theory (DFT) calculations have become commonplace in the characterisation, design and prediction of materials, but in most conventional implementations, suffer from a scaling problem: the computing time cost increases with the cube of the number of atoms. Conquest [1] (<http://ordern.github.io>) is a first principles electronic structure code that can perform DFT calculations that scale linearly with the number of atoms, and as such, is capable of almost ideal parallel efficiency even when using more than 200,000 cores to deal with million-atom systems. This includes Born-Oppenheimer molecular dynamics (MD) in the micro-canonical and canonical [2] ensembles, and extended-Lagrangian Born-Oppenheimer MD [3] which includes electronic degrees of freedom in the equations of motion, solving fundamental problems involving time-reversibility.

Constant pressure MD is necessary because it is a closer match to experimental and planetary interior conditions than constant volume, and it facilitates the modeling of polymorphic phase transitions. Moreover, it is often difficult to choose the correct volume when modeling complex amorphous or biological systems, especially in cases when the calculated density does not match the experimental density. In this talk, I will discuss the implementation of isobaric-isothermal (NPT) molecular dynamics in the context of a linear scaling DFT code, Conquest. We demonstrate that efficient and robust NPT simulations are now possible for systems containing 10,000+ atoms, using simulations of silica in the Earth's mantle as an example.

[1] D. R. Bowler, T. Miyazaki, *Rep. Prog. Phys.* **75**, 36503 (2012).

[2] T. Hirakawa, T. Suzuki, D. R. Bowler, T. Miyazaki, *J. Phys.: Condens. Matter* **29**, 405901 (2017).

[3] M. Arita, D. R. Bowler, T. Miyazaki, *J. Chem. Theor. Comput.* **10**, 5419 (2014).

## Ion-induced electron emission from 2D materials

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Large amounts of potential energy initially stored in a highly charged ion (HCI) can get released upon ion impact on a substrate. Charge exchange and deexcitation of the ion lead to excitation and subsequent emission of target electrons into vacuum once the ion approaches the target's surface. Therefore, potential electron emission above the surface as well as kinetic electron emission (as a result of momentum transfer from the projectile to target electrons) inside the material take place. We measure the number of emitted electrons due to one single ion impact by means of electron emission statistics. Ion-induced electron emission has been studied for a various number of bulk materials with different properties (e.g. work function and energy band gap) [1,2]. Here, we use now freestanding 2D materials and find that the amount of emitted electrons (about 100 electrons/ion) does not increase with increasing interaction time (slower ions) in contrast to bulk material s. This might result from a limited reservoir of electrons at the impact area. We compare the ion-induced electron emission from a single layer of semi-metallic graphene and a monolayer of semiconducting MoS<sub>2</sub> to the emission from bulk targets.

[1] F. Aumayr, H. Kurz, et al., *Physical Review Letters* **71**, 1943-1946 (1993).

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## Modelling of hydrogen retention in tungsten based on *ab initio* calculations

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In this contribution, we present a model of hydrogen retention in tungsten as a result of the interaction with plasma. The model describes how the retention is governed by accumulation at dislocations, nucleation of critical stable clusters and their growth. In a nutshell, the interaction of H with dislocation lines was computed using Density Functional Theory. A mechanism for the nucleation and growth of bubbles comprises of the following stages: (1) interstitial H atoms getting trapped at dislocation lines due to favourable energetics; (2) their very fast one dimensional migration along the dislocation core because of low migration energies; (3) the growth of multiple H atom clusters, eventually resulting in the creation of a vacancy jog on the dislocation core. Implementation of these mechanisms in a simple Rate Theory (RT) model allowed reaching relevant trends in agreement with experimental evidence.



## Higher-Order Topological Defect States in Insulators

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Bulk-boundary correspondence is a key feature of topological insulators (TI) [1], which allows to relate the properties of the bulk electronic structure to the existence of localized electronic states at the boundaries of the crystal. In particular it is well known, that the  $Z_2$  invariant, being a pure bulk property of a 3D TI indicates existence of gapless (metallic) surface states. In recent years there have tremendous advances in identifying new topological insulating phases in crystalline solids, including 3D "higher-order topological insulators" (HOTIs)[2], which exhibit gapped 2D surfaces (unlike TIs) but gapless 1D hinges. On the other hand, numerous proposals have linked the anomalous electronic states bound to defects in crystalline solids[3] to the bulk electronic structure of pristine crystals[4,5] In particular, it was demonstrated [4,5] that screw dislocations and edge disclinations in weak TIs can bind anomalous 1D electronic states.

In this work, we extend the classification of topological electronic defect states, by relating the topological properties of specific planes in momentum space to the charges bound to the ends of line defects in crystals. In particular we show, that a screw or line dislocation with Burgers vector  $\vec{B}$  binds higher-order "end states" (HENDs) when the electronic structure of a plane defined by  $\vec{B} \cdot \vec{k} = \pi$  is classified as a 2D obstructed atomic limit [6] of a fragile topological phase [7]. We support our findings by numerical calculations. Using the DFT-calculated bandstructure we show that the plane  $k_z = \pi/a$  ( $a$  being the lattice parameter) of the bulk Brillouin zone of SnTe is a 2D obstructed atomic limit. With use of a tight binding model we show that the end of an edge dislocation with Burgers vector  $\vec{B} = (0, 0, a)$  has a bound state, while no 1D states are bound along the dislocation.

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## Deep learning in aid to high resolution AFM experiments

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Atomic Force Microscopy (AFM) offers unique capability to analyze structure of molecules and solid surfaces with atomic resolution. Constant demand on development of new materials and studying chemical processes made it widespread experimental tool in the recent years. Nevertheless preparation of advanced AFM experiments (e.g. attachment of CO tip) still require great expertise and suffer from lack of automation. Interpretation of three-dimensional molecular structures from AFM images is hindered by distortions and artifacts due to CO bending and molecular movement. Automation of those operations and introducing expert tools based on machine learning (ML) can help to speed up experimental process and provide additional information for analysis of unknown molecular mixtures. We are developing methodology to apply ML image-recognition models to several such tasks, including recognition of 3D molecular structures and assessing quality of CO functionalized tips. Resolving those tasks we consider different aspects of deep learning models training on both simulated and experimental AFM data.

## In-situ growth of MoS<sub>2</sub> Nanoparticles on Reduced Graphene Oxide Aerogels for Efficient HER Electrocatalysis

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Recently, the composites of the two-dimensional (2D) transition metal dichalcogenides (TMDs) and the carbonaceous nanomaterials of graphene have attracted much attention in the clean and renewable hydrogen energy [1,2]. As the cost-effective, non-noble earth-abundant and stable electrocatalysts, the composites of MoS<sub>2</sub> and Graphene are promising to replace the expensive noble Pt and its alloys in hydrogen evolution reaction (HER) to solve the energy crisis and relevant pollution concerns [3-5]. In this work, we report a facile one-pot hydrothermal method to synthesize stable hybrid 3D porous reduced graphene oxide (rGO) dispersed by MoS<sub>2</sub> nanoflowers, in which MoS<sub>2</sub> nanoflowers tightly and well-decorated on 3D porous rGO aerogels. All the above factors make the hybrid aerogels are characterized by excellent optimization in adsorption and electrocatalytic hydrogen evolution reaction (HER) with a low overpotential of 0.130 V, a small Tafel slope of 39 mV/decade and large current density. This study potentially provides new avenues for designing more efficient transition metal sulfides and carbonaceous nanomaterials as the non-metallic hybrid catalytic for hydrogen energy.

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## Growth and Characterization Thin Films on Graphene in Ultra High Vacuum

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Heterostructures of two-dimensional materials have recently drawn great interest. In a building-block approach the electronic properties of a compound can be tailored with its constituent materials and their interactions. At the University of Vienna we installed a manipulation chamber for physical vapour deposition within our ultra high vacuum (UHV) transport system. This allows for evaporation onto standard-sized TEM-grids and the transport to our Nion UltraSTEM 100 aberration corrected scanning transmission electron microscope in UHV conditions for analysis. Here we present our setup and first data on silicon, gold and indium in situ evaporation, as well as differences to conventional set-ups with intermediate exposure to an uncontrolled atmosphere.

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