DCAFM
Retreat 2024

2024

29-31 January 2024, Laa an der Thaya

Contents

About

Venue

Therme Laa

Location

The hotel is located in Laa an der Thaya, roughly 1.5 hours from Vienna, and close to the Czech border.

Address: Thermenplatz 3, 2136 Laa a. d. Thaya, Austria

Opening hours

Therme Laa: 09:00-22:00
Hotel spa area: 07:00-22:00

Organizing committee

Christiane Maria Losert-Valiente Kroon	christiane.losert@univie.ac.at
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Timetable

CT: Contributed Talk, IT: Invited Trainer

Monday, January 29

9:40		Meeting Point: Train Station Wien Floridsdorf, Platform 4 (Train REX2)	
9:56–11:30		Travel to Laa/Thaya, Check-in at Hotel Therme Laa	
12:00–13:00		Lunch	
13:30–17:30	IT	**Michael Gordian** Career Coaching	Workshop 1 - Input
16:30–18:00		PI Meeting	
18:00–19:00		Dinner	
		Chair: Andrea Angeletti	
19:00–19:20	CT	**Carsten Speckmann** Supervisor: Jani Kotakoski	Title: Electron-beam-induced vacancy-adatom-complexes in mono- and bilayer phosphorene
19:20–19:40	CT	**Ivan Novikau** Supervisor: Sofia Kantorovich	Title: Wobbling in Nanogel Hydrodynamic and Magnetic Responses
19:40–20:00	CT	**Roman Staňo** Supervisor: Christos Likos	Title: Ring polymers … but with a twist
20:00–open		Team Meeting – Students & PIs	

Tuesday, January 30

8:00–9:00		Breakfast	
9:00–13:00	IT	**Michael Gordian/DCAFM Faculty** Career Coaching	Workshop 2 - Mock Interviews
13:00–14:00		Lunch	
14:00–17:30		**Social Program: Hiking with Alpacas/Enjoy the Spa**	
18:00–19:00		Dinner	
		Chair: Ivan Novikau	
19:00-19:20	CT	**Clara Freytag** Supervisor: Thomas Pichler	Title: Carbon nanotube and carbyne hybrid structures
19:20–19:40	CT	**Martin Unzog** Supervisor: Georg Kresse	Title: X-ray absorption spectra of carbon nanotubes using the Bethe-Salpeter equation
19:40–20:00	CT	**Lukas Brandfellner** Supervisor: Alexander Bismarck	Title: Extrapolating drag reduction as function of Reynolds number and degradation
20:00–open		**Pub Quiz - Host: Carsten Speckmann**	

Social Program

Spa

Spa at Therme Laa or
the Hotel Therme Laa spa
Facilities: Pool, Sauna, thermal spa
Details: https://www.therme-laa.at

Hiking with Alpacas

Place: Josefsweg 4, 2130 Siebenhirten. (Follow the signs to Schlösslgasse),
Transportation: 30 min by taxi from Hotel Therme Laa
Clothes: Winter clothes (No special equipment is needed)
Contact: +43 664 5651 106 /
info@alpakazucht-siebenhirten.at

Wednesday, January 31

Time		Speaker	Title
8:00–9:00		Breakfast	
9:00–9:30		Check-out	
Chair: Ksenija Simonović			
9:30–9:50	CT	**Lukáš Kývala** Supervisor: Christoph Dellago	Title: Unsupervised identification of local atomic environment from atomistic potential descriptors
9:50–10:10	CT	**Andrea Angeletti** Supervisor: Cesare Franchini	Title: Defects, materials, properties and dynamics via machine learning accelerated molecular dynamics calculations
10:10–10:30	CT	**Dóra Vörös** Supervisor: Leticia González	Title: Unveiling Surface Interactions of Push-Pull Functionalized Stilbene: Adsorption and Absorption on Silica Glass
10:30–10:50		Coffee Break	
Chair: Roman Staňo			
10:50–11:10	CT	**Joselyn Benalcázar Jaramillo** Supervisor: Paola Ayala	Title: Optical properties of zig-zag single-walled carbon nanotubes
11:10–11:30	CT	**Ksenija Simonović** Supervisor: Markus Arndt	Title: Exploring molecular properties using far-field matter-wave diffraction
11:30–12:30		Wrap-up	
12:30–13:30		Lunch	
13:45		Departure to Vienna	

List of Abstracts – Talks

Electron-beam-induced vacancy-adatom-complexes in mono- and bilayer phosphorene

C. Speckmann,[1,2] *D. Lamprecht*,[1,3] *C. Mangler*,[1] *F. Herterich*,[1] *and J. Kotakoski*[1]

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Phosphorene, a puckered two-dimensional allotrope of phosphorus, has peaked a lot of interest in recent years due to its potential especially for optoelectronic applications due to its layer-number-dependant direct bandgap and strongly bound excitons [1]. However, detailed experimental characterization of its intrinsic defects as well as its defect creation characteristics under electron irradiation are scarce [2,3]. We report on the creation and stability of a variety of defect configurations under 60 kV electron irradiation in mono- and bilayer phosphorene including the first experimental reports of stable adatom-vacancy-complexes which have previously only been discussed in theory [4]. Displacement cross section measurements in bilayer phosphorene yield a value of 7.7 +/- 1.4 barn with an estimated lifetime of adatom-vacancy-complexes of 19.9 +/- 0.7 s, while some of them are stable for up to 68 s under continuous electron irradiation. As defects can drastically alter the properties of materials, increasing or diminishing the performance of devices, understanding these key properties is necessary not only for fundamental research, but also applications. These results will help to improve the understanding of the wide variety of defects in phosphorene, their creation and their stability, which might open up new possibilities for defect engineered phosphorene devices.

References
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[2] Yao et al., 2D Mater. 8, 025004 (2020)
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[4] Vierimaa et al., Nanoscale 8, 7949-7957 (2016)

CT

Wobbling in Nanogel Hydrodynamic and Magnetic Responses

Ivan Novikau,[1] _and Sofia Kantorovich_[1,2]

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Magnetic Nanogels (MNGs) are versatile soft materials widely used in drug delivery due to their compatibility with external magnetic fields. Recent research has focused on incorporating magnetic nanoparticles (MNPs) into nanogels for targeted drug delivery, enhanced uptake by tumor cells, and advancements in medical imaging and therapy. This study utilizes molecular dynamics (MD) simulations and the Lattice-Boltzmann (LB) scheme to investigate the magnetic controllability of MNGs. Specifically, we explore the effective transfer of MNP torque to the polymer matrix, providing insights into guiding MNGs through the circulatory system. We quantitatively measure the magnetic susceptibility of MNGs and evaluate the influence of an external magnetic field on their viscoelastic properties at the suspension scale, with a specific focus on the dynamic modulus.

Ring polymers … but with a twist

Roman Staňo,[1] _Davide Michieletto_[2], _Ján Smrek_[1], _Christos N. Likos_[1]

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DNA, certain classes of biofilaments or graphene nanoribbons are all examples of materials with a ribbon topology. Ribbons exhibit both torsional and bending stiffness. When the two ends of a ribbon are connected together, like for instance in DNA plasmids, neither bending nor torsional stiffness can be mechanically fully relaxed. Instead, the corresponding degrees of freedom are coupled, transforming bending into torsion and vice versa, while keeping their combined topological signature - the degree of supercoiling - constant. The geometry and topology of a ribbon can be described using concepts of twist and writhe, the former characterizing the rotation and winding of the plane of the ribbon, while the latter is connected to self-crossings of the ribbon in its projection. The aim of our study is to find out how can one control the competition between twist and writhe, and the resultant geometry of ring ribbon polymers. Inspired by recent experimental studies, we explore two strategies for such a topological control: one utilizing chemical reaction equilibrium, the other one using non-equilibrium mechanical manipulation by molecular engines.

Carbon nanotube and carbyne hybrid structures

Clara Freytag,[1] _Weili Cui_,[1,2] _Lei Shi_,[2] _Emil Parth_,[1] _Christin Schuster_,[1] _and Thomas Pichler_[1]

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Carbyne is the elusive carbon allotrope with sp^1 hybridized carbon, leading, to an infinite linear chain of carbon atoms. Theoretically, it is a true 1D nanomaterial with unique electronic and mechanical properties, for example it is predicted to be the world's strongest material [1] and the strongest Raman scatterer [2]. In the past years, carbyne was successfully synthesized inside carbon nanotube hosts [3] and the growth mechanisms have since been well understood [4,5]. In this work I will present advances on understanding the temperature dependent Raman signal using a state-of-the art in-situ cryostat set-up. We have also improved the theoretical model of the Raman modes of confined carbyne using DFT. As a next step, we aimed at creating hybrid structures containing carbyne. Here I will present results on single-walled carbon nanotubes filled with nitrogen doped precursors and the synthesis of double-walled carbon nanotubes and carbyne. I will also present results on coaxial structures of carbon nanotubes with boron nitride nanotubes synthesized with chemical vapor deposition [6], with the aim of growing carbyne inside the nanotube cable.

References
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X-ray absorption spectra of carbon nanotubes using the Bethe-Salpeter equation

Martin Unzog,[1] *, Alexey Tal,*[2] *, Pedro Melo,* [2], *Ryosuke Senga,* [3], *Kazu Suenaga,* [3], *Thomas Pichler,* [4]*, and Georg Kresse* [5]

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Single-walled carbon nanotubes (SWCNTs) are cylinders formed from sheets of graphene. Due to their one-dimensional nature, they have unique mechanical, optical and transport properties that make them interesting for current and future device applications. Characteristic of the one-dimensional nature of single-walled carbon nanotubes (SWCNTs) are the Van Hove singularities (VHS) visible in their electronic ground state density of states (DOS). Recently, it was suggested that the VHSs and the fine structure seen in X-ray absorption spectra of isolated SWCNTs are closely related. This relationship was established for the (6,5) SWCNT by superimposing a suitably shifted DOS on the X-ray absorption spectrum and by identifying a peak in the fine structure with a particular VHS. In this work, we model X-ray absorption spectra of isolated SWCNTs using methods based on density functional theory and many-body perturbation theory. In particular, we use a variant of the supercell core-hole method and a recent implementation of the Bethe-Salpeter equation for x-ray spectra. Modeled and experimental spectra of isolated SWCNTs are compared with their DOS and it is demonstrated that the relationship between VHS and absorption edge peaks generally does not hold. The discrepancies are caused by the coupling of the core state to multiple VHSs. By studying the core-exciton wavefunctions of a graphene supercell, we will explain that this coupling to multiple VHSs is induced by the periodic boundary conditions imposed on the SWCNT.

Extrapolating drag reduction as function of Reynolds number and degradation

Lukas Brandfellner,[1,2] _Hans Werner Müller,_[1] _and Alexander Bismarck_[1,2]

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Polymeric drag reduction (DR) is of great interest for liquid transport applications as well as for improving the understanding of the interplay of molecular dynamics and turbulent flow. Depending on the Reynolds number (Re) of the flow different DR regimes can be distinguished. At low and high Re DR becomes independent of molecular properties of the polymer and either the friction factor f coincides with f of a Newtonian fluid (low Re) or follows a universal maximum drag reduction (MDR) asymptote (high Re). The onset of DR, the approach of the MDR, and the transition regime in between are governed by concentration, molecular weight and molecular weight distribution of the polymer additive. The relation with the molecular weight is bidirectional as polymers degrade in DR application, leading to a decrease in molecular weight. These interactions are essential for understanding the polymer turbulence interplay and the mechanism of DR. We studied drag reduction and degradation of polyacrylamide with different initial molecular weight in a pilot scale flow facility called ViEDRA (Vienna Experiment for Drag Reducing Agents). ViEDRA studies were accompanied by size exclusion chromatography, which provided the development of the molecular weight distribution of the applied polymers. Variation of Re in the flow experiments at selected stages of degradation allowed us to describe f as function of Re and degradation and to extrapolate f along these two variables. The extrapolation provided DR in the whole transition regime as well as the onset of DR and the approach of the MDR asymptote.
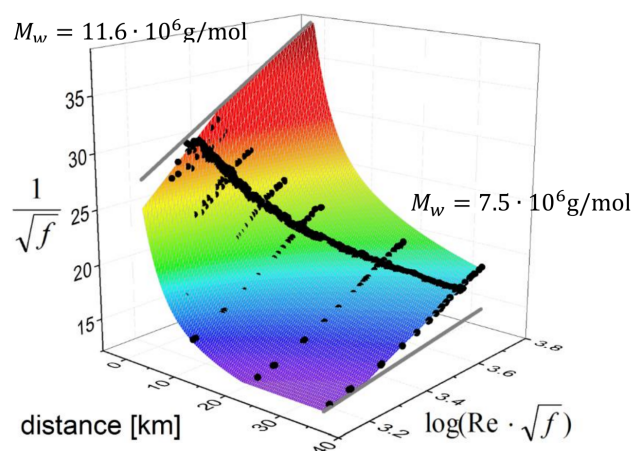
Figure 1: Experimental (black) and extrapolated friction factor of PAAm with varying Re. The molecular weight decreases with flow distance due to polymer degradation in turbulent flow.

Unsupervised identification of local atomic environment from atomistic potential descriptors

Lukáš Kývala,[1] *and Christoph Dellago*[1]

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Machine learning potentials significantly accelerate molecular dynamics simulations, allowing us to model much longer time spans and larger systems. However, this opens the challenge of post-analysis for certain simulations, such as studying the mobility of defects or phase growth, like nucleation. In these cases, visual analysis is not practical, and it is necessary to develop specific analyses for each material. These are usually accompanied by additional calculations of order parameters, which are not trivial to design and can incur significant computational overhead for very long simulations. It is much simpler to leverage atomistic potential descriptors, which describe local chemical environment, and have already been computed for energy and force predictions during simulation. In my talk, I will demonstrate how atomistic potential descriptors can provide information about the local atomic environment. Utilizing the PaCMAP dimensional reduction algorithm, we can not only count hopping events of monovacancy in phosphorene but also unequivocally determine the hopping mechanism. All of this can be achieved in an unsupervised mode without providing prior knowledge and with minimal hyperparameter tuning. I will further showcase the application of these methods in the analysis of silicon.

Defects materials properties and dynamics via machine learning accelerated molecular dynamics calculations

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Defects, omnipresent in materials, exert a profound influence on electronic properties, notably through point defects like vacancies or impurities. Employing Density Functional Theory (DFT) calculations via VASP, allow to explor the impact of such defects on electronic structures. Machine learning-accelerated molecular dynamics simulations have been performed as well, facilitating the modeling of defect transition mechanisms, offering insights into their dynamic behavior. DFT database has been used to train an High Dimensional Neural Network potential, leading to a common publication focused to the study of phosphorene monovacancy, merging into divacancy. Beyond phosphorene, the research ventured into the exploration of superconductive ternary hydrides, specifically N-doped lutetium hydride. By utilizing the bayesan on-the fly machine learning force fields (MLFF) accelerated molecular dynamics, we scrutinized the emergence and stability of molecular hydrogen within these compounds, expanding the applicability of the technique. Therefore, the overall investigation unveiled the intricate dynamics of defect coalescence and also showcased the adaptability of the innovative computational methods to model the behavior of defects in different materials. In response to novel experimental measurements, the current research has evolved to characterize a novel type of defect in both phosphorene monolayer and bilayer configurations. Furthermore, the MLFF and a fine-tuned CHGNet universal pretrained potential are been used to study the hydrogen diffusion in magnesium and alloy.

CT

Unveiling Surface Interactions of Push-Pull Functionalized Stilbene: Adsorption and Absorption on Silica Glass

**Dóra Vörös**,[1,2] **Felix Proché**, [1], **Andrea Angeletti**,[2,3] **Cesare Franchini**,[3] **Sebastian Mai**,[1] _and Leticia González_[1]

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In our research, we explore how amorphous silica surfaces influence the photophysical and photochemical properties of 4-(N,N-dimethylamino)-4'-nitrostilbene (DANS), a stilbene derivate known for its photoisomerization and notable fluorescence emission. Changing the environment, like the introduction of different solvents, can affect its absorption spectra and even modify the ratio between photoisomerization and fluorescence. Previous studies have demonstrated that how the interaction with microplastics can lead to significant changes in the fluorescence emission. [1] The goal of this study is to understand the interactions between DANS and the glass surface and investigate the changes in the photophysical and photochemical properties of DANS due to that interaction. In the initial phase, we conducted optimization calculations with plane wave density functional theory on different orientations on the glass surface. [2] Following this, we assessed the interaction energies and examined the optimized geometries to determine the most favorable orientations. In order to gain a better understanding of the various orientations, we applied a range of techniques including analyzing charge density differences, clustering, and employing multiple linear regression. The results suggest that the hydrogen bonds between the nitro group of DANS and the OH group of the surface is very important. Furthermore, the involvement of the π-system plays a surprisingly significant role in the energy interaction, thereby enhancing the stability of the molecule on the surface. To gain insights into light-induced phenomena, we conducted calculations with time dependent density functional theory in the excited states and analyzed the absorption spectra of the gas phase as well as various orientations on the silica surface. We applied wave function analysis methods to observe changes in excitation in comparison to DANS in gas phase. Additionally, we utilize wave function overlap calculations to gain a deeper understanding of the similarities and differences between the wave function of DANS on glass and the wave function of DANS in the gas phase. Through an examination of the acquired absorption spectra, it was discovered that the hydrogen bond with the nitro group also leads to the most significant changes in the absorption spectra.

References
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Optical properties of zig-zag single-walled carbon nanotubes

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Optical spectroscopy is an extremely powerful tool to study single-walled carbon nanotubes (SWCNT), which are peculiar nanostructures that exhibit physical properties strictly depending on the geometrical arrangement of their atoms. They have distinct electronic absorption and emission transitions, therefore the composition of bulk or mixed composition SWCNT samples can be inspected by optical spectroscopy providing access to diameter and chiral angle distributions. Perfect structures, as theoretically predicted, exhibit specific spectral values. However, a number of effects can deviate spectral responses obtained experimentally from those theoretically expected. This is why significant research is still invested in making single chirality clean samples or, at least, producing large scales of metallicity sorted material. Despite great advances on highly efficient post-synthesis purification and sorting methods for SWCNTs, accurate studies on single chirality batches still differ from the theory. Depending on the species, one can expect to observe specific types of vibrations at certain frequencies as well as unique intensities along the carbon nanotubes spectrum. Diameter and chirality theoretical tendencies are expected to be observed with a variety of close-diameter single chirality nanotubes. I will show our progress on the use of a highly efficient two-step sorting method optimized to extract zig-zag SWCNT chiralities and sorting the tubes with the smallest possible diameter range (0.7-0.9 nm). This is extremely useful for further studies on the structure-dependent optical properties. Raman spectroscopy, optical absorption and photoluminescence have been primarily used for this study.

Exploring molecular properties using far-field matter-wave diffraction

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Light gratings are a highly versatile and powerful tool in matter-wave diffraction. While in atom interferometry the laser wavelength can be tuned close to an atomic resonance, allowing for outstanding control over internal and external degrees of freedom, the complex internal structure hampers this approach in high-mass molecular and cluster interference. Instead, optical gratings in molecular interferometry build on high power continuous wave (cw) laser light at 532 nm [1–3] or pulsed UV lasers [4, 5]. Realizing cw gratings in the UV was so far impeded by the lack of lasers with sufficient output power and fast degradation of UV optics in high vacuum [6]. Here we demonstrate single-grating diffraction of molecular matter-waves at a 266 nm cw grating. Compared to diffraction at 532 nm gratings, this leads to a wider spacing of the diffraction orders, allowing us to explore more massive molecules compared to previous far-field measurements. In particular, we focus on applications for quantum-assisted measurements, using diffraction images to extract molecules' intrinsic optical properties such as polarizability and absorption cross section at 266 nm. The deep UV diffraction grating paves the way for studying photo-physical and photo-chemical processes of biologically and technologically relevant molecules in matter- wave diffraction. At the same time, it explores new grating mechanisms for high-mass cluster interferometry and complex biomolecules, such as depletion gratings based on single photon induced photocleavage [7]. In the second part of the talk, we revisit previous work done on diffracting polar organic molecules on material gratings [8], which suffer from dephasing due to interactions with the grating. In current experiments we compare several polar and potentially polar molecules, working towards characterising and ranking their dipole moments. Furthermore, we show that these experiments pave the way towards assessing molecular structures via matter- wave diffraction experiments [9].

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List of Participants

Michael Gordian		Communication coach
Markus Arndt	Ksenija Simonović	Quantum Nanophysics
Alexander Bismarck	Lukas Brandfellner	Polymer and Composites Engineering
Christoph Dellago	Lukáš Kývala	Computational Statistical Mechanics
	Andrea Angeletti	Computational Quantum Materials
Georg Kresse	Martin Unzog	Computational Materials Physics
	Dóra Vörös	Institute of Theoretical Chemistry
Sofia Kantorovich	Ivan Novikau	Dipolar Soft Matter
Jani Kotakoski	Carsten Speckmann	Physics of Nanostructured Materials
Christos Likos	Roman Staňo	Soft Matter Theory and Simulation
Paola Ayala	Joselyn Benalcázar Jaramillo	Tailored Hybrid Structures
Thomas Pichler	Clara Freytag	Electronic Properties of Materials

Partner Institutions and Sponsors

The Doctoral College Advanced Functional Materials (DCAFM) is a topical college in the Vienna Doctoral School in Physics (VDSP). The faculty of the DCAFM consists of members of the Faculties of Physics and Chemistry of the University of Vienna with complementary backgrounds in diverse fields of materials science. Research in Hierarchical Design of Hybrid Systems (HiDHyS) focuses on three specific classes of hybrid materials: van der Waals heterostructures, carbon nanomaterials and macromolecular aggregates and their mechanical, electronic and magnetic properties. The project HiDHyS (project number DOC85) is funded by the FWF Austrian Science Fund.