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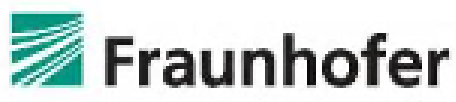
**RU Workshop 2023**

**Reducing complexity of nonequilibrium systems**

***Book of Abstracts***

**19. – 22.09.2023**

**Freiburg im Breisgau**



**universität freiburg**

## Organisation

Gerhard Stock, Spokesperson

Email: [gerhard.stock@physik.uni-freiburg.de](mailto:gerhard.stock@physik.uni-freiburg.de)

Michael Thoss, Deputy Spokesperson

Email: [michael.thoss@physik.uni-freiburg.de](mailto:michael.thoss@physik.uni-freiburg.de)

Simone Ortolf, Coordination

Email: [simone.ortolf@physik.uni-freiburg.de](mailto:simone.ortolf@physik.uni-freiburg.de)

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## Imprint

FOR 5099 / Institute of Physics

University of Freiburg

Hermann-Herder-Straße 3

D - 79104 Freiburg

## General Information

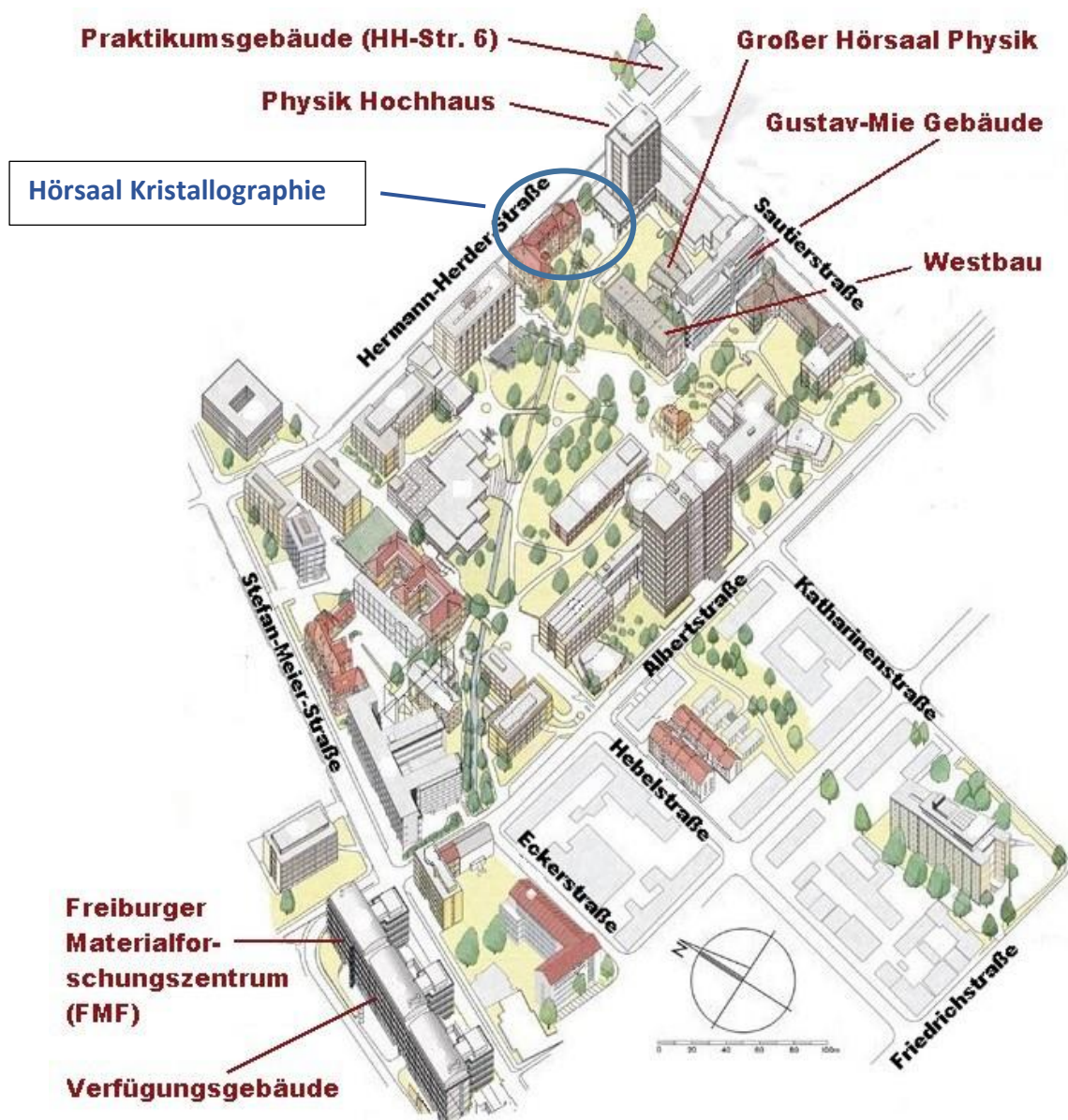
### Duration

Tuesday, September 19, 2023, 08:45 am – Friday, September 22, 2023, 01.00 pm

### Location

Institute of Physics - Hermann-Herder-Str. 3 - 79104 Freiburg

Lectures: Hörsaal Kristallographie – Hermann-Herder-Str. 5 - 79104 Freiburg



## Meals & Drinks

Breakfast: For our invited guest speakers accommodated in The Alex Hotel & Motel One Hotel, breakfast will be included.

Coffee Breaks: During the scientific programme, coffee breaks in the morning and in the afternoon will be available at the entrance area of the lecture hall.

Lunch: During lunch breaks, a buffet will be provided in the Common Room (11<sup>th</sup> floor) of the physics high-rise (Physik Hochhaus).

Conference Dinner: Following our excursion, we will have our conference dinner at Waldrestaurant St. Valentin on Thursday, 21.09.m from 6:30 pm.

Address:

Waldrestaurant St. Valentin  
Valentinstraße 100  
79100 Freiburg im Breisgau  
<https://www.sanktvalentin.eu/>

## Excursion - Kybfelsen

On Thursday afternoon, our hike to the Kybfelsen will take place, starting in Freiburg Günterstal. The approx. 2-hour hike of medium difficulty takes us past various vantage points and the St. Lioba monastery garden. The hike ends at the Restaurant St. Valentin, where we will have our conference dinner. You will receive further information in advance of the hike on Thursday.



(View from Kybfelsen, photo by sistjala.de)

INFORMATION - Freiburg im Breisgau

Freiburg im Breisgau was founded in 1120 by *Konrad and Duke Berthold III of Zähringen*. Because of its position at a junction of both trade routes from the Mediterranean Sea of the North Sea and the Rhine and Danube rivers, the city prospered and gained attraction from both traders and artisans. In ca. 1200, during the rule of the last *Duke of Zähringen*, construction began of the Münster, the big cathedral in the middle of the city and one of the most famous landmarks of Freiburg. The building was officially consecrated at December the 5th. 1513. While the building itself is being used by them, it does not actually belong to the Catholic Church. Rather it is still owned by the citizens of Freiburg, which is a rarity for churches in Europe. Roughly, 45 years earlier, in 1457, after founding the first university in Austrian-Habsburg territory in Vienna, the Habsburg dynasty founded the *Albert-Ludwigs-University*. It is the fifth-oldest university in Germany. Today, it is seen as one of the country's top universities and has gained international reputation. The city of Freiburg itself has many different unique details and secrets to find, should one go exploring. One of them is quite openly visible in some parts of the town. Framing the streets of the inner city, one of the oldest still standing parts of Freiburg, are small channels, sometimes decorated with colorful little boats. They are called "Bächle", which means "small creek" in the south-german dialect of the region allegedly, every person, who accidentally steps into one of them will marry a citizen of Freiburg, so remember... Beware of the Bächle!

**Gestalten Sie Ihren Stadtrundgang**

1 Alte Wache	17 Münsterbauhütte	33 Museen	41 Getheshäuser	49 Universität	57 Bertoldbrunnen	65 Parkhäuser	73 Schlossberg
2 Basler Hof	18 Rathaus	34 Archäologisches Museum „Colombischlöche“	42 Adelhäuser Kirche	50 Alte Universität	58 Karlsplatz	66 Bahnhofgarage	74 Schwabentor
3 Erzbischöfliches Ordinariat	19 Schwabentor	35 Augustinermuseum	43 Martinikirche	51 Universitätsbibliothek (im Bau befindlich)	59 Fahrradstation mobile	67 Volksbank	75 Am Martinstor
4 Erzbischöfliches Palais	20 Stadtbibliothek	36 Faunmuseum	44 Synagoge	52 Universitätskirche	60 Schlossbergbahn	68 Am Bahnhof	76 Uni-Kollegiengebäude
5 Gerichtslaube	21 Stadtgarten	37 Museum für Neue Kunst	45 Kultur	53 Universitätszentrum	61 Siegesdenkmal	69 Untertinden	77 Schwarzwald City
6 Haus zum Wolfisch	22 Zum Roten Bären	38 Naturmuseum	46 Jazzhaus	54 Theater	62 Hauptbahnhof	70 Konzerthaus	78 Kotteck
7 Historisches Kaufhaus		39 Uniseum	47 Konzerthaus	55 Theater im Marienbad	63 Busbahnhof	71 Kunstverein	79 Zähringer Tor
8 Martinstor		40 Wentzingerhaus	48 Planetarium	56 Theater	64 Post	72 Museum für Stadtgeschichte	80 Karlsruher
		41 Zinnfigurenklaue	49 Wollgrabentheater			73 Theater	81 Busparkplätze
							74 Karlsplatz
							75 Stadtgarten
							76 Schreiberanlage

## Program

Tuesday, September 19, 2023

<b>SESSION 1</b>	Chair: <b><i>Joachim Dzubiella</i></b>
08:45 a.m.	<u>Gerhard Stock</u> Welcome and Introduction
09:00 a.m.	<u>Pratyush Tiwary</u> Search for meaning in data with dynamics based priors
09:40 a.m.	<u>Christoph Dellago</u> Machine learning for rare event simulations
10:20 a.m.	<u>Sebastian Milster</u> Tracer friction and memory in polymer networks
11:00 a.m.	<b>Coffee Break</b>
11:30 a.m.	<u>Udo Seifert</u> Concepts from stochastic thermodynamics for model-free inference
12:10 p.m.	<u>Sofia Sartore</u> You Get What You Give: Feature selection in Markov state modelling
12:30 p.m.	<u>Miriam Jäger</u> Path Separation of Non-Equilibrium MD trajectories
12:50 p.m.	<b>Lunch</b> Common Room, Physics High-rise, 11 <sup>th</sup> floor
<b>SESSION 2</b>	Chair: <b><i>Sabine Klapp</i></b>
02:00 p.m.	<u>Lydéric Bocquet</u> Water and ion transport in 1D and 2D nanochannels, from carbon memories to quantum friction
02:40 p.m.	<u>Michael Moseler</u> Understanding dry friction of covalent materials sliding on epitaxial graphene
03:20 p.m.	<u>Lars Pastewka</u> Elasticity, viscoelasticity, and plasticity of amorphous materials
04:00 p.m.	<b>Coffee Break</b>
04:30 p.m.	Postersession

## Program

Wednesday, September 20, 2023

<b>SESSION 3</b> Chair: <i>Michael Thoss</i>	
09:00 a.m.	<u>Yoshitaka Tanimura</u> Numerically “exact” simulations of a quantum Carnot cycle: Analysis using thermodynamic work diagrams
09:40 a.m.	<u>Samuel Rudge</u> Electronic Friction, Current-Induced Forces, and a Semiclassical Approach to Charge Transport in Molecular Nanojunctions
10:20 a.m.	<u>Dvira Segal</u> The Reaction Coordinate method in quantum dynamics and thermodynamics
11:00 a.m.	<b>Coffee Break</b>
11:30 a.m.	<u>Walter Strunz</u> Open quantum system dynamics and thermodynamics from a global state point of view
12:10 p.m.	<u>Moritz F. Richter</u> Measuring Information Flow in Phase Space: A Classical and Quantum Perspective
12:50 p.m.	<u>Graziano Amati</u> Signatures of non-Markovianity in dissipative-driven quantum dynamics
01:10 p.m.	<b>Lunch</b> Common Room, Physics High-rise, 11 <sup>th</sup> floor
<b>SESSION 4</b> Chair: <i>Heinz-Peter Breuer</i>	
02:30 p.m.	<u>Roland Netz</u> Projection Methods for Non-Markovian Non-Equilibrium Systems
03:10 p.m.	<u>Tanja Schilling</u> Where intuition about Brownian particles fails
03:50 p.m.	<u>Thomas Speck</u> Tracking dissipation across scales in active matter
04:30 p.m.	<b>Coffee Break</b>
	Free afternoon & evening

## Program

Thursday, September 21, 2023

<b>SESSION 5</b>	Chair: <b><i>Dmitrii E. Makarov</i></b>
09:00 a.m.	<u>Xuhui Huang</u> Non-Markovian Dynamic Models for Studying Protein Conformational Changes
09:40 a.m.	<u>Christine Peter</u> Dimensionality reduction and clustering in multiscale simulations of conformational free energy landscapes
10:20 a.m.	<u>Gerhard Stock</u> Nonequilibrium Approach to Allosteric Communication
11:00 a.m.	<b>Coffee Break</b>
11:30 a.m.	<u>Alessandro Laio</u> Identifying informative distance measures in high-dimensional feature spaces
12:10 p.m.	<u>Thorsten Koslowski</u> Biological charge transfer far from equilibrium: electron migration and entropically driven proton dislocation
12:50 p.m.	<b>Lunch</b> Common Room, Physics High-rise, 11 <sup>th</sup> floor
<b>SESSION 6</b>	Chair: <b><i>Christine Peter</i></b>
02:00 p.m.	<u>Paolo Carloni</u> Metadynamics Simulations for the Estimation of Ligand Binding Kinetics
02:40 p.m.	<u>Steffen Wolf</u> Predicting Protein–Ligand (Un)Binding Kinetics with Biased MD Simulations and Langevin Equation-Based Coarse-Graining of Dynamics
03:20 p.m.	<b>Coffee Break</b>
04:00 p.m.	Excursion
06:30 p.m.	Conference Dinner Waldrestaurant St. Valentin



## Program

Friday, September 22, 2023

<b>SESSION 7</b>	Chair: <b><i>Christoph Dellago</i></b>
09:00 a.m.	<u>Kurt Kremer</u> Playing with entanglements to structure polymer materials
09:40 a.m.	<u>Sabine Klapp</u> Patterns in active fluids on various scales
10:20 a.m.	<u>Kerstin Falk</u> Boundary lubrication: from molecular dynamics to rheological models
11:00 a.m.	<b>Coffee Break</b>
11:30 a.m.	<u>Dmitrii E. Makarov</u> Information-theoretical analysis of single-molecule trajectories
12:10 p.m.	<u>Michael Thoss</u> Closing

## **Abstracts**

-

## **Lectures**

## Search for meaning in data with dynamics based priors

Pratyush Tiwary and Dedi Wang

University of Maryland

While representation learning has been central to the rise of machine learning and artificial intelligence, a key problem remains in making the learnt representations meaningful. For this the typical approach is to regularize the learned representation through prior probability distributions. However such priors are usually unavailable or ad hoc. To deal with this, we propose a dynamics-constrained representation learning framework. Instead of using predefined probabilities, we restrict the latent representation to follow specific dynamics, which is a more natural constraint for representation learning in dynamical systems. Our belief stems from a fundamental observation in physics that though different systems can have different marginalized probability distributions or free energy profiles, they typically obey the same underlying dynamics, such as Newton's and Schrodinger's equations. We validate our framework for different systems including a real-world fluorescent DNA movie dataset. We show that our algorithm can uniquely identify an uncorrelated, isometric and meaningful latent representation. Additionally, we will explore other methods for incorporating physics into learning low-dimensional representations and discuss the strengths and weaknesses of these different approaches.

## Machine learning for rare event simulations

Christoph Dellago

Faculty of Physics, University of Vienna

The microscopic dynamics of many condensed matter systems occurring in nature and technology is dominated by rare but important barrier crossing events. Examples of such processes include nucleation at first order phase transitions, chemical reactions and the folding of biopolymers. The resulting wide ranges of time scales are a challenge for molecular simulation and numerous simulation methods have been developed to address this problem. Recently, machine learning methods have been proposed as a powerful way to further enhance such simulations. In my talk, I will discuss various machine learning approaches based on deep neural networks to sample rare reactive trajectories and identify the collective variable needed for the construction of low-dimensional models capturing the microscopic mechanism.

## **Tracer friction and memory in polymer networks**

Sebastian Milster, Christoph Widder, Fabian Koch, Tanja Schilling,  
and Joachim Dzubiella

Institute of Physics, University of Freiburg

This work studies the dynamics of small molecules in a fluctuating polymeric environment. While the long-time diffusion is widely understood, the control of the highly correlated dynamics on shorter time scales is key to efficient selective particle transport, particularly, under nonequilibrium conditions. We employ implicit-solvent Langevin simulations of regular, tetrafunctional bead-spring polymer networks containing spherical tracer solutes in very high dilution. We analyze the dynamics based on autocorrelation functions and friction memory kernels for different network densities, tracer sizes, and interaction strengths. We recover the long-term transport coefficients from different methods and describe the characteristic short-time memory of the polymer network and the tracers by damped harmonic oscillations as a function of the system parameters. This reveals the dynamic coupling between the solutes and the polymer environment, allows for a convenient interpolation of the memory kernels, and efficient simulation of large systems based on the generalized Langevin equation.

## Concepts from stochastic thermodynamics for model-free inference

Udo Seifert

Institute for Theoretical Physics, University Stuttgart

Stochastic thermodynamics provides a universal framework for analyzing nano- and micro-sized non-equilibrium systems. Prominent examples are single molecules, molecular machines, colloidal particles in time-dependent laser traps and biochemical networks. Thermodynamic notions like work, heat and entropy can be identified on the level of individual fluctuating trajectories. They obey universal relations like the fluctuation theorem.

Thermodynamic inference as a general strategy uses consistency constraints derived from stochastic thermodynamics to infer otherwise hidden properties of non-equilibrium systems. As a paradigm for thermodynamic inference, the thermodynamic uncertainty relation discovered in 2015 provides a lower bound on the entropy production through measurements of the dispersion of any current in the system. Likewise, it quantifies the cost of temporal precision for biomolecular processes and provides a model-free bound on the thermodynamic efficiency of molecular motors and microscopic heat engines.

Generalizations allow us to apply it to time-dependently driven systems like the unfolding of proteins under mechanical force. Waiting time distributions between observable events yield even better bounds on entropy production and the topology and driving affinity of the underlying network.

## **You Get What You Give: Feature selection in Markov state modeling**

Sofia Sartore, Daniel Nagel, Georg Diez, and Gerhard Stock

Institute of Physics, University of Freiburg

Features selection, i.e., the choice of suitable input coordinates, is arguably the most crucial step when building a dynamic model such as a Markov state model (MSM). That is, to obtain meaningful and easily interpretable results, it is essential to use features that are representative of the mechanism and facilitate the structural distinction of the different conformational states of the considered process. Various techniques exist, that allow to make an educated first guess of suitable features and to reduce the dimensionality of the problem to a small set of descriptive collective variables. Using the folding process of the villin headpiece and the functional motion of T4 lysozyme as examples, we introduce the correlation-based analysis MoSAIC which uses a community detection algorithm allowing to discard coordinates that are unrelated to the motion of interest and to identify clusters of features that represent the same biomolecular process. We also highlight how a poor choice of input features can hamper a valid MSM ('garbage in, garbage out').

## Path Separation of Non-Equilibrium MD trajectories

Miriam Jäger and Steffen Wolf

Institute of Physics, University of Freiburg

The understanding of dynamics and free energy landscapes of ligand association and dissociation from proteins is limited by the timescales of these transitions. To enhance the sampling of such rare transitions we enforce ligand unbinding from a protein by applying dissipation-corrected targeted MD (dcTMD) simulations, which enforce a moving distance constraint along a pre-chosen reaction coordinate. As dcTMD analysis is dependent on the pathway taken by the ligand, we require a clustering of unbinding trajectories according to the pathways taken. We here present an approach for such a pathway clustering based on ligand-protein contacts using Leiden community detection with the constant Potts model as an objective function.



## Water and ion transport in 1D and 2D nanochannels, from carbon memories to quantum friction

Lydéric Bocquet

Ecole Normale Supérieure - CNRS, 24 rue Lhomond, Paris, France

The emerging field of nanofluidics explores the molecular mechanics of fluids. This world of infinitesimal fluidics is the frontier where the continuum of fluid dynamics meets the atomic nature of matter, or even its quantum nature. Nature fully exploits the fluidic oddities at the nanoscale and it is capable of breath-taking technological feats using a fluidic circuitry made of multiple biological channels, such as ionic pumps, proton engines, ultra-selective pores, stimuable channels, ... A major challenge at stake is to harness the strange properties of fluid transport at nanoscale to reproduce or mimic some of these functionalities.

In this talk, I will discuss various experimental and theoretical results that we obtained recently on the far-from-equilibrium transport of water and ions in ultra-confinement, both in 1D nanotubes and 2D channels obtained by van der Waals assembly. I will in particular discuss the water-carbon couple, which highlights a variety of exotic transport properties. I will focus on two such phenomena: the emergence of memory in quasi-two-dimensional water channels and the development of elementary ion-based computing, with basic forms of Hebbian learning [1,2]; and the nearly frictionless flows of carbon nanotubes and its quantum roots [3,4,5].

I will conclude by briefly discussing how such nanoscale emerging phenomena can be exploited to develop technological innovations for water and energy.

### References

- [1] “Long-term memory and synapse-like dynamics of ionic carriers in two-dimensional nanofluidic channels”, P. Robin, T. Emmerich, A. Ismail, A. Nigues, Y. You, G.-H. Nam, A. Keerthi, A. Siria, A.K. Geim, B. Radha, L. Bocquet, *Science* 379, (2023)161-167.
- [2] “Modeling of emergent memory and voltage spiking in ionic transport through angström-scale slits”, P. Robin, N. Kavokine, and L. Bocquet, *Science* 373, (2021)687–691.
- [3] “Massive radius-dependent flow slippage in single carbon nanotubes” E. Secchi, S. Marbach, A. Niguès, D. Stein, A. Siria and L. Bocquet, *Nature* 537 (2016) 210.
- [4] “Fluctuation-induced quantum friction in nanoscale water flows”, N. Kavokine, M.-L. Bocquet and L. Bocquet, *Nature* 602, (2022) 84-90.
- [5] “Strong electronic winds blowing under liquid flows on carbon surfaces”, M. Lizée, et al., *Physical Review X* 13, (2023) 011020.

## Understanding dry friction of covalent materials sliding on epitaxial graphene

Michael Moseler

Fraunhofer IWM

&

Institute of Physics, University of Freiburg

Epitaxial graphene on SiC(0001) exhibits superlow friction due to its weak out-of-plane interactions. Friction force microscopy with silicon and diamond tips shows an abrupt increase of friction by one order of magnitude above a threshold normal force. Density-functional tight-binding simulations of silica against epitaxial graphene suggest that this wearless high-friction regime involves an intermittent  $sp^3$  rehybridization of graphene at contact pressure exceeding 10 GPa. The simultaneous formation of covalent bonds with the silica tip's surface and the underlying SiC interface layer establishes a third mechanism limiting the superlow friction on epitaxial graphene, in addition to dissipation in elastic instabilities and in wear processes. [1] Tight-binding simulations of H/OH-terminated amorphous carbon sliding against epitaxial graphene reveal different friction regimes. Above 15 GPa normal pressure, hydrogen transfer to the graphene occurs, followed by amorphization of the graphene at normal pressure above 20 GPa. We explore the super-low sliding regime, where no bonds form between the tip and the graphene, through classical molecular dynamics with a specially designed non-reactive force field for functionalized amorphous carbon tips in contact with graphene. Low frictional forces are obtained for hydrogenated surfaces, while hydroxylation induces high frictional forces that are inconsistent with the experiments. Consequently, oxygen end groups must be of the ether type.

### References

[1] B. Szczefanowicz et al., Formation of intermittent covalent bonds at high contact pressure limits super-low friction on epitaxial graphene, *Phys. Rev. Research* **5**, L012049 (2023)

## **Elasticity, viscoelasticity, and plasticity of amorphous materials**

Ibrahim Ghanem, Jan Griebner, Richard Jana, Lars Pastewka

Department of Microsystems Engineering, University of Freiburg, Germany

Disordered materials respond to external deformation by internal relaxation. In a small-strain linear-response limit, these nonaffine atomic displacements are reversible but they serve to couple long-wavelength macroscopic deformation modes to short-wavelength vibrations. Beyond linear response, deformation is irreversible, leading to what has been termed the shear-transformation zone. This talk shows how computer simulations of nonaffine displacement in ultrastable model glasses, amorphous silicon and amorphous carbon yield insights into viscoelasticity and plasticity of disordered materials.

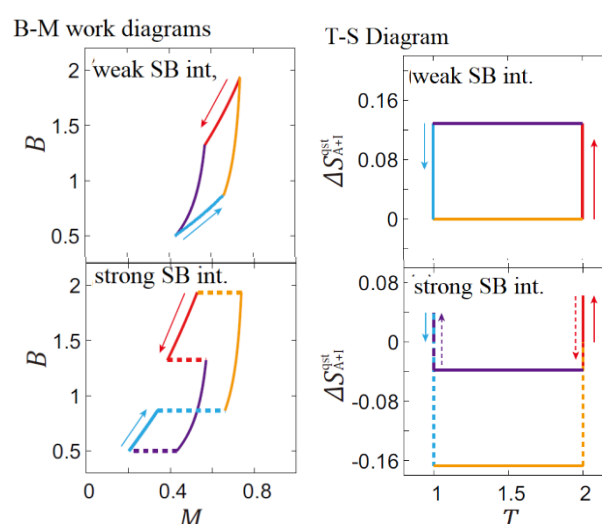
## Numerically “exact” simulations of a quantum Carnot cycle: Analysis using thermodynamic work diagrams

Yoshitaka Tanimura

Department of Chemistry, Kyoto University

<http://theochem.kuchem.kyoto-u.ac.jp/members/tanimura.htm>

Numerically accurate simulations of a quantum Carnot engine were conducted in a non-perturbative and non-Markovian system-bath (SB) coupling regime based on the hierarchical equations of motion (HEOM) theory.[1] The model includes time-dependent external fields for the subsystems controlling the isothermal and isentropic processes ( $B(t)$ ) and for the SB interactions controlling the transition between isothermal and isentropic processes ( $A_k(t)$  for  $k=1$  and  $2$ ). By regarding quasi-static work as free energy, we compute conjugated thermodynamic variables ( $M(t)$  and  $D_k(t)$ ) to analyze the simulation results using thermodynamic work diagrams for the first time. We find that the maximum efficiency is achieved in the quasi-static case and is determined solely by the temperatures of the baths, regardless of the SB coupling strength, which is a numerical manifestation of Carnot's theorem. Moreover, based on rigorous numerical results, we also show that the thermodynamic laws are partially satisfied even in non-equilibrium regime. A possibility of measuring free energy in a quantum regime by means of multidimensional spectroscopies will be also discussed.



*B-M and T-S diagrams for 8 strokes quantum Carnot cycle modeled by a two-level system coupled with hot and cold heat baths with weak and strong time-dependent SB interactions. (from Ref. [1])*

[1] S. Koyanagi & Y.T. JCP.157, 084110 (2022); <https://doi.org/10.1063/5.0107305>

[2] S. Koyanagi & Y.T. JCP157,014104(2022); <https://doi.org/10.1063/5.0093666>

## Electronic Friction, Current-Induced Forces, and a Semiclassical Approach to Charge Transport in Molecular Nanojunctions

Samuel Rudge, Christoph Kaspar, Martin M'ack, Robin Grether, and Michael Thoss

Institute of Physics, University of Freiburg, Hermann-Herder-Strasse 3, 79104  
Freiburg, Germany

When molecules move near a metal surface, electronic excitations even at very low energies can couple to nuclear motion and prevent a simple description with adiabatic potential energy surfaces. One popular way to describe such nonadiabatic transitions is electronic friction, which provides a damping mechanism for vibrational motion via electron-hole pair creation. Theories based on including these processes have proven historically successful in scenarios where the nuclear motion is essentially classical but where electronic states do not have well-separated energies, such as in the calculation of the lifetimes of vibrational modes of molecules adsorbed on a surface [1] or in the scattering of molecules off metal surfaces [2].

Recently, the idea of electronic friction has also permeated the field of molecular electronics. In these systems, a molecule is contacted to two metal electrodes and driven out of equilibrium with a finite voltage bias. In this context, electronic friction arises as a current-induced force acting on the relevant vibrational modes of the molecule, and it connects directly to junction stability, as the positive-definiteness and symmetry of the friction tensor are not guaranteed out of equilibrium [3]. We have developed a method for calculating electronic friction and other current-induced forces based on the numerically exact hierarchical equations of motion (HEOM) approach [4]. Given that HEOM can be applied to a wide variety of systems and in a broad parameter regime [5], this approach to electronic friction and the resulting semiclassical equations of motion for vibrational motion represents one of the most general approaches to current-induced forces in molecular junctions to date. In this contribution, we first introduce the method and then discuss its range of validity application to several problems in the context of transport in nanostructures, such as waterwheel-type nuclear motion, molecules with modes of very different frequencies, and current-induced bond rupture.

[1] M. Head-Gordon and J. C. Tully, *J. Chem. Phys.* 103, 10137–10145 (1995)

[2] P. Spiering and J. Meyer, *J. Phys. Chem. Lett.* 9, 7, 1803–1808, (2018)

[3] W. Dou and J. E. Subotnik, *J. Chem. Phys.* 148, 230901 (2018)

[4] S. L. Rudge, Y. Ke, and M. Thoss, *Phys. Rev. B* 107, 115416 (2023)

[5] Y. Tanimura, *J. Chem. Phys.* 153, 020901 (2020)

## The Reaction Coordinate method in quantum dynamics and thermodynamics

Dvira Segal

Department of Chemistry, University of Toronto, Canada

I will describe our recent advances to the reaction coordinate method, turning it from a numerical tool to a semi-analytical framework capable to distill the impact of strong system-bath coupling effects in open quantum systems. Our reaction-coordinate polaron transform (RCPT) approach, which is based on two exact transformations of the Hamiltonian followed by its controlled truncation, ends with a new Hamiltonian with a weakened coupling to the environment. This new effective Hamiltonian mirrors the initial one, except that its parameters are dressed by the system-bath couplings. After presenting the RCPT method, I will illustrate it on "canonical" problems of quantum thermalization and charge and energy transport at the nanoscale. I will further offer benchmarking against other popular (perturbative and numerically-exact) methods.

### References:

N. Anto-Sztrikacs, A. Nazir, and D. Segal, Effective-Hamiltonian Theory of Open Quantum Systems at Strong Coupling, PRX Quantum 4, 020307 (2023)

## **Open quantum system dynamics and thermodynamics from a global state point of view**

Walter Strunz

Institute for Theoretical Physics, TU Dresden

Irreversible quantum (thermodynamic) processes are ubiquitous in nature and offer challenges both from an applied and fundamental point of view. Important practical (computational) and conceptual issues are still open. Fundamentally, quantum irreversibility arises as subdynamics of a unitary global evolution. In this contribution we employ such a global state point of view for the study of the dynamics of a quantum heat engine, allowing us to investigate in detail the various energetic contributions and changes during each cycle.

## **Measuring Information Flow in Phase Space: A Classical and Quantum Perspective**

Moritz F. Richter and Heinz-Peter Breuer

Institute of Physics, University of Freiburg, Germany

Exchange of information between an open quantum system and its environment, especially the backflow of information to the system associated with quantum notions of non-Markovianity, is a widely discussed topic for years now. Usually the information flow is quantified by the increase of suitable distance measures between two initial states of the open quantum system at hand. However, the same idea can also be used to identify information backflow in classical systems and their dynamics in phase space. In the talk we will discuss how information backflow can be measured for the dynamics of open quantum systems and how this can be translated to classical dynamics in phase space. We will then explain the relations between both quantum and classical measures in case of continuous variable quantum systems and demonstrate how the one transforms to the other for a suitably defined quantum-to-classical transition.



## **Signatures of non-Markovianity in dissipative-driven quantum dynamics**

Graziano Amati and Tanja Schilling

Institute of Physics, University of Freiburg, Germany

Dissipation is a fundamental physical process occurring in dynamical systems which classify as 'open', i.e. interacting with an external environment. Dissipative dynamics are often labeled as non-Markovian, in contrast to Markovian memory-less processes. It is to date controversial how to optimally quantify non-Markovian effects in quantum mechanics, and which measures of dissipation are at best capable of capturing all the relevant properties of the system of interest with minimal computational cost.

The trace distance is a metric between quantum states which quantifies their mutual distinguishability, and allows to infer a measure of dissipation from it. In the talk I will discuss the numerically exact dynamics of a dissipative-driven qubit, obtained by integrating the hierarchical equations of motion. I will apply the trace-distance approach to measure non-Markovianity and the occurrence of stochastic resonances in the system. The analysis will be compared with other approaches, including the study of the Nakajima-Zwanzig generalized quantum master equation and of nonadiabatic transition rates.

## Projection Methods for Non-Markovian Non-Equilibrium Systems

Roland R. Netz

Department of Physics, Free University Berlin, Arnimallee 14, 14195 Berlin, Germany

Most physical systems are interacting many-body systems, one typically describes their kinetics in terms of low-dimensional reaction coordinates. The dynamics of such reaction coordinates is governed by the generalized Langevin equation (GLE), an integro-differential stochastic equation, and involves a memory function, which describes how the reaction coordinate dynamics depends on its previous values. The GLE is thus an intrinsically non-Markovian description of the dynamics of a system in terms of coarse-grained variables. We have recently introduced a novel hybrid projection scheme that allows to extract the GLE parameters from time series data in a form that is convenient for analytic and numerical treatments [1] and have shown that memory effects are significant for protein folding [2,3].

Non-equilibrium effects are characterized by slowly relaxing transient variables and can be described by a time-dependent Hamiltonians, in fact, non-equilibrium systems typically exhibit pronounced memory effects. Two systematic approaches for such systems will be discussed: Using an appropriate projection, a non-equilibrium formulation of the GLE is presented. As an alternative approach, data filtering is shown to lead to modified GLEs that are particularly useful for the treatment of time series data from non-physical sciences.

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Cihan Ayaza, Lucas Tepper, Florian N. Brünig, Julian Kappler, Jan O. Daldrop, Roland R. Netz  
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[3] Fast protein folding is governed by memory-dependent friction

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Proc. Natl Acad. Sci. (2023, in press), <https://arxiv.org/abs/2208.13842>

## **Where intuition about Brownian particles fails**

Tanja Schilling

Institute of Physics, University of Freiburg

We discuss the generalized Langevin equation under the action a time-dependent external force. Using a projection operator formalism, we show under which conditions a fluctuation-dissipation theorem can be produced, and we point out where analogies to Newtonian mechanics break down.

## Tracking dissipation across scales in active matter

Thomas Speck

Institute for Theoretical Physics IV, University of Stuttgart

Systems that are steadily driven away from thermal equilibrium are characterized by a non-vanishing entropy production rate. Active matter encompasses a wealth of autonomous non-equilibrium systems characterized by local microscopic dissipation. How this dissipation shapes the large-scale collective behavior in synthetic colloidal and living cellular active matter is of current interest, in particular when aiming to extract useful work. When going to a coarser scale, microscopic information is lost and typically only lower bounds on the dissipation rate can be formulated. I will present our recent work how dissipation can be tracked across scales for motile active matter, i.e., suspensions of self-propelled particles. Starting from a microscopic model including explicit fuel molecules, the model of active Brownian particles, and in the next step the effective hydrodynamic equations, can be constructed while fully accounting for the dissipation. Some applications will be discussed.

# Non-Markovian Dynamic Models for Studying Protein Conformational Changes

Xuhui Huang

University of Wisconsin-Madison

Protein's dynamic transitions between metastable conformational states play an important role in numerous biological processes. Markov State Model (MSM) built from molecular dynamics (MD) simulations provides a useful approach to study these complex dynamic transitions, but it is challenging to build truly Markovian models due to the limited length of lag time (bound by the length of relatively short MD simulations). In this talk, I will introduce our recent work on developing non-Markovian dynamic models based on the Generalized Master Equation (GME) theory that encodes the dynamics in a generally time-dependent memory kernel, whose characteristic decay time scale corresponds to the kernel lifetime. We show that GME methods can greatly improve upon Markovian models by accurately predicting long timescale dynamics using much shorter MD trajectories on complex conformational changes. I will also present our newly developed algorithm, the Integrative GME-based Neural Network (IGMEnet), which can accurately identify the slow CVs of biomolecular dynamics. Our IGMEnet algorithm is distinct from popular deep-learning approaches, such as VAMPnet and SRVnet, which assume Markovian dynamics. Instead, IGMEnet is built on the GME theory. Its key innovation is the development of a novel loss function that corresponds to the integrals of memory kernels. By optimizing this loss function in encoder deep-neural networks, we demonstrate that our IGMEnet algorithm can effectively identify the slow CVs involved in the folding of the FIP35 WW-domain with high accuracy. Furthermore, we tested IGMEnet on a more complex conformational change, specifically the clamp opening of a bacterial RNA polymerase (a system consisted of over 540K atoms), where the sampling from all-atom MD simulations is limited. Our results demonstrate that IGMEnet greatly outperforms SRVnet, which is based on Markovian dynamics and may result in disconnected dynamics along the identified CVs. We expect that the GME-based methods hold promise to be widely applied to study functional dynamics of proteins.

## **Dimensionality reduction and clustering in multiscale simulations of conformational free energy landscapes**

Christine Peter

University of Konstanz

Simulating long-timescale or non-equilibrium processes often requires a combination of scales that starts from an atomistic level of resolution and involves coarse graining in space or time. Learning meaningful low-dimensional representations of the sampled conformational phase space and identifying conformational states is of increasing importance both for the development and assessment of spatially coarse grained as well as for kinetic models. I will present examples how machine-learning and network-based analysis methods can be used to investigate and characterize interactions in different biomolecular systems. Moreover, I will show how low-dimensional representations enable us to assess the consistency of the sampling in different models, to go back and forth between simulation scales and ultimately to enhance and improve the sampling of the systems.

## Nonequilibrium Approach to Allosteric Communication

Gerhard Stock

Institute of Physics, University of Freiburg

Allostery represents a fundamental mechanism of biological regulation, which is mediated via long-range communication between distant protein sites. While little is known about the underlying dynamical process, recent time-resolved infrared spectroscopy experiments on photoswitchable PDZ domains have indicated that the allosteric transition occurs on multiple timescales. Employing extensive nonequilibrium molecular dynamics simulations, here a time-dependent picture of the allosteric communication in PDZ domains is developed. The simulations reveal that allostery amounts to the propagation of structural and dynamical changes that are genuinely nonlinear and may occur in a nonlocal fashion. A dynamic network model is constructed that illustrates the hierarchy and exceeding structural heterogeneity of the process. In compelling agreement with experiment, three physically distinct phases of the time evolution are identified, describing elastic response (0.1 ns), inelastic reorganization ( $\sim 100$  ns) and structural relaxation (1  $\mu$ s). Issues such as the similarity to downhill folding as well as the interpretation of allosteric pathways are discussed.

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Phil. Trans. B 373, 20170187 (2018).

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J. Phys. Chem. Lett. 13, 9862 (2022).

## Identifying informative distance measures in high-dimensional feature spaces

Alessandro Laio

International School for Advanced Studies (SISSA), Trieste, Italy

Real-world data in biochemistry, material science and beyond typically contain a large number of features that are often heterogeneous in nature, relevance, and also units of measure. When assessing the similarity between data points, one can build various distance measures using subsets of these features. Finding a small set of features that still retains sufficient information about the dataset is important for the successful application of many statistical learning approaches. We introduce a statistical test that can assess the relative information retained when using two different distance measures, and determine if they are equivalent, independent, or if one is more informative than the other. This test can be used to identify the most informative distance measure and, therefore, the most informative set of features, out of a pool of candidates. The approach can be used to identify the most appropriate set of collective variables in molecular systems and to infer causality in high-dimensional dynamic processes and time series.



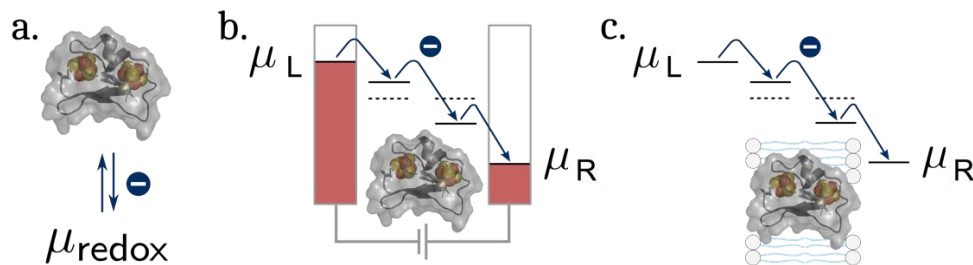
## Biological charge transfer far from equilibrium: electron migration and entropically driven proton dislocation

Mike Castellano<sup>1</sup>, Jetmir Haxhija<sup>1</sup>, Felix Guischar<sup>1</sup>, Christoph Kaspar<sup>2</sup>,  
Michael Thoss<sup>2</sup>, Thorsten Koslowski<sup>1</sup>

<sup>1</sup>Institut für Physikalische Chemie, Universität Freiburg, Albertstr. 21, 79104 Freiburg

<sup>2</sup>Institut für Physik, Hermann-Herder-Str. 3, 79104 Freiburg

Potential differences for electron transfer through biopolymers or in bio-nano setups can amount to several 100 mV. We describe these situations by Pauli-Master equations that are based on Marcus' theory of charge transfer between self-trapped electrons and that obey Kirchhoff's current law. We present analytical and numerical current-potential curves and electron populations for multi-site model systems and biological electron transfer chains. Based on these, we provide empirical rules for electron populations and chemical potentials along the chain. The Pauli-Master mean-field results are validated by kinetic Monte Carlo simulations. We discuss the biochemical and evolutionary aspects of our findings.



**Figure 1.** Cartoon representation of charge transfer scenarios. Redox-active protein in equilibrium with its environment (a.), non-equilibrium transfer through a protein bridging two metallic leads (b.) or a lipid bilayer (c.). Protein atoms as grey spheres, chromophore atoms in color.

In the vital respiratory complex I, electron transfer is followed by protein-quinone unbinding, which in turn triggers proton dislocation against a pH gradient. We estimate the entropic contributions to this process in lipid bilayers and obtain an entropy drive of up to 12 kcal/mol. We suggest an entropic zipper model and discuss it in the context of the bioenergetics and the structure of complex I.

## **Metadynamics Simulations for the Estimation of Ligand Binding Kinetics**

Paolo Carloni

Institute for Advanced Simulation (IAS), Forschungszentrum Jülich GmbH

The dissociation rate ( $k_{\text{off}}$ ) associated with ligand unbinding events from proteins is an important parameter in drug design. Many major advancements in molecular simulations allow to predict  $k_{\text{off}}$  values. Here we will present some metadynamics enhanced sampling simulations from our lab on cytoplasmatic proteins and membrane receptors. We will conclude the talk with a perspective from high-performance computing and machine learning to potentially improve such predictions.

## **Predicting Protein–Ligand (Un)Binding Kinetics with Biased MD Simulations and Langevin Equation-Based Coarse-Graining of Dynamics**

Steffen Wolf

Institute of Physics, University of Freiburg

The prediction of drug–target binding and unbinding kinetics that occur on time scales between milliseconds and several hours is a prime challenge for molecular dynamics simulation approaches. To compute (un)binding dynamics and the related affinity constants, here we present a combination of dissipation-corrected targeted MD and temperature-boosted Langevin equation simulations. Using simulations of a few nanoseconds individual length, the fully atomistic data is rationalized in the form of only two profiles, which are the free energy  $\Delta G(x)$  and friction  $\Gamma(x)$ . Using these profiles in Langevin equation-based simulations allows to access dynamics on time scales of seconds to hours, which is several magnitudes beyond the capabilities of atomistic MD approaches. Analyzing the kinetics-defining transition states  $\Delta G(x)$  and  $\Gamma(x)$  for a range of pharmaceutically relevant target–drug complexes, we find that the transition barrier height usually is related to the rupture of enthalpic interactions such as salt bridges and hydrogen bonds, while friction corresponds to the solvation of a ligand and the protein binding site. Lastly, we demonstrate how small structural changes between two compounds already can lead to drastically altered unbinding paths, highlighting the challenges in the computation of (un)binding kinetics.

## Playing with entanglements to structure polymer materials

Kurt Kremer

Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128, Mainz, Germany  
(kremer@mpip-mainz.mpg.de)

Entanglements are known to dominate the rheological properties of long chain polymer melts and dense solutions. Their properties and consequences lead to the generally accepted and well established reptation/tube model, which is at the basis of our understanding of many properties and processes. However, beyond analysing their effects and understanding the very nature of entanglements, one also can take the approach to use them to manipulate and structure materials. The talk will give a few such examples ranging from melts of non-entangled to very long, highly entangled polymer systems. By appropriately mapping chemical chain lengths onto idealized bead spring models one can (semi-) quantitatively compare simulation and experiment and predict new materials. Based on predictions from simulations we recently prepared stable nanoporous polymer films just by mechanical deformation. Furthermore, we applied a new data driven approach to determine the glass transition temperature of polymer melts and (ultra) thin films.

Free Standing Dry and Stable Nanoporous Polymer Films Made through Mechanical Deformation  
HP Hsu, MK Singh, Y Cang, H Thérien-Aubin, M Mezger, R Berger, I Leiberwirth, G Fytas, K Kremer  
Adv. Sci. 2023, 2207472

Data-driven identification and analysis of the glass transition in polymer melts  
A Banerjee, HP Hsu, K Kremer, O Kukhareenko  
ACS Macro Lett. 2023, 12, 679–684

Glass transition of disentangled and entangled polymer melts: Single-chain-nanoparticles approach  
MK Singh, M Hu, Y Cang, HP Hsu, H Thérien-Aubin, K Koynov, G Fytas, K Landfester, K Kremer  
Macromolecules 2020, 53, 7312-7321

## Patterns in active fluids on various scales

Sabine Klapp

<sup>1</sup>*Institute of Theoretical Physics, TU Berlin, Hardenbergstrasse 36,10623 Berlin*

In this talk we will discuss recent results on the collective behavior and pattern formation of active systems exhibiting vortices and chiral motion, focusing on the performance of (and connections between) different levels of theoretical description. The first example concerns suspensions of microswimmers exhibiting mesoscale turbulence. We employ a continuum-theoretical approach which can be derived microscopically [1] and allows for a quantitative modelling of experiments [2]. Considering systems in periodic arrays of obstacles, we explore the transition from a vortex state to mesoscale turbulence. We find an intriguing similarity with a second-order phase transition characterized by critical exponents in the 2D Ising universality class and an effective temperature that can be related to a particle-dependent quantity, that is, the motility [3]. The second example concerns systems with intrinsic chirality (circle swimmers) and non-reciprocal alignment coupling. The resulting collective dynamics involves, beyond flocking and motility-induced phase separation, also frustrated states induced by non-reciprocity. We investigate the large-scale behavior of these systems using a mean-field-like continuum theory and linear stability analysis [2]. In addition, we present particle-based simulations of the underlying Langevin equations. The latter allow us to characterize the complex dynamics microscopically, and to assess the role of correlations.

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## **Boundary lubrication: from molecular dynamics to rheological models**

Kerstin Falk

Fraunhofer IWM

The design process of lubricated sliding contacts in mechanical machinery is heavily relying on the Reynolds equation, which is a thin-film approximation of the Navier-Stokes equations. While providing an excellent description of hydrodynamic lubrication, the Reynolds equation is expected to fail under so-called boundary lubrication conditions. Boundary lubrication occurs especially in highly loaded tribological contacts with local pressures up to several Gigapascal, and is characterized by lubricant film heights of a few nanometers and below, which also implies very high shear rates. Under these extreme conditions, the rheological response of the lubricant to the sliding motion may not be describable with the equilibrium transport coefficients due to confinement and/or non-linear effects. One established way to investigate the validity of continuum equations on the nanoscale is via the comparison to molecular dynamics simulation results. In this talk, results from MD shearing simulations of oil lubricated tribological model systems including surface roughness are discussed. It is shown that the validity of the Reynolds description can be extended into the boundary lubrication regime by introducing non-linear constitutive laws for the lubricant's shear viscosity and wall slip. Finally, some aspects of the microscopic origin of the non-linear response of the viscosity and the slip velocity are discussed.

## Information-theoretical analysis of single-molecule trajectories

Dmitrii E Makarov

Department of Chemistry and Oden Institute for Computational Engineering and Sciences

University of Texas at Austin

Experimental single-molecule studies have opened a new window into the elementary biochemical steps, function of molecular machines, and cellular phenomena. The information contained in single-molecule trajectories is however often underutilized in that oversimplified models such as one-dimensional diffusion or one-dimensional random walk are used to interpret experimental data. In this talk I will discuss several practical approaches through which much finer details of single-molecule dynamics, such as conformational memory, static disorder, and entropy production (even in the absence of overall directional motion) can be deduced from an analysis that is similar to Shannon's analysis of printed English; in particular, this method relates conformational memory to the information-theoretical compressibility of single-molecule signals.

## Poster Abstracts

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### List of presented Posters

1. **Ahmed Ali** - Allosteric Signaling in Photoswitchable PDZ3 Domain
2. **Mike Castellano** - High voltage rock'n'roll: a theoretical approach to protein electron transfer far from equilibrium.
3. **Georg Diez** - Correlation-Based Feature Selection Unveils Functional Dynamics in Proteins
4. **Emanuel Dorbath** - Log-periodic oscillations as result of hierarchical dynamics in proteins
5. **Ibrahim Ghanem** - Plasticity in amorphous carbon as a stress-assisted chemical reaction
6. **Nils Göth** - Active Responsive Colloids
7. **Christoph Kaspar** - Nonadiabatic vibronic effects in single-molecule junctions: A theoretical study using the hierarchical equations of motion approach
8. **Lars Kruse** - Adsorption characteristics of novel star polymers as lubricant additives
9. **Martin Mäck** - Current-Induced Bond Rupture in Molecular Junctions: A Semi-Classical Langevin Approach Based on Electronic Friction
10. **Daniel Nagel** - Benchmarking Markov State Models: A Case Study on the Folding of HP35
11. **Kiyoto Nakamura** - Rigorous numerical method beyond the Markov, Born and perturbative approximations: simulations of gate sequences of qubits in presence of noise
12. **Sven Pattloch** – Mean-field models for the chemical fueling of transient soft matter states
13. **Irene Ada Picatoste** - Witnessing non-Markovianity in quantum Brownian motion by quasi-probability distributions in phase-space
14. **Riley Preston** - Applications of Landauer's blowtorch effect in nonequilibrium transport through molecular junctions
15. **Rudolf Smorka** - Nonequilibrium dynamics in spin valve heterojunctions
16. **Franziska Stief** - Shear thinning behavior of PAO4 with ZDDP additive in bulk liquid
17. **Mohammad Zarshenas** - Exploring Dry Friction of Amorphous Carbon on Epitaxial Graphene: Insights and Observations



## **Allosteric Signaling in Photoswitchable PDZ3 Domain**

*Studied by Nonequilibrium MD Simulations and Markov State Models*

Ahmed Ali and Gerhard Stock

Institute of Physics, University of Freiburg

Allostery is one of the most important mechanisms for biomolecular regulation. Generally, it involves a perturbation such as a binding event at one side of a macromolecule to affect another distant functional site. However, how such a perturbation propagates through the protein in detail is still not well understood. To establish a minimal allosteric model system, the third PDZ domain (PDZ3) of the postsynaptic density-95 (PSD-95) protein has been considered. The PDZ3 domain binds to the C-terminus of target proteins and regulates the signal propagation in PSD-95. In addition to the common and conserved central  $\beta$ -sheets and two  $\alpha$ -helices present in all PDZ variants, PDZ3 contains a third C-terminal  $\alpha$ -helix ( $\alpha_3$ -helix) that packs against the  $\beta$ -sheet at a considerable distance to the ligand binding pocket.

In this work, we aim for a detailed understanding of the microscopic dynamics of allosteric communication between  $\alpha_3$  and the ligand binding pocket. In addition, we explicitly aim at finding intraprotein changes appearing on the same time scales as found in recent time-resolved IR spectroscopic experiments. Consequently, we perform direct nonequilibrium molecular dynamics simulations of PDZ3, by attaching a photowswitch at the allosteric site ( $\alpha_3$ ) and mimicking the initial cis  $\rightarrow$  trans photoisomerization of the azobenzene photoswitch via a potential-energy surface switching method, in order to mimik the allosteric process and observe it in real time. We characterize the  $\alpha_3$ -switched response by correlation and timescales analysis, which reproduces experimental timescales accurately. Furthermore, we construct Markov state models to describe the structural evolution of the allosteric process of PDZ3.

Nonequilibrium Modeling of the Elementary Step in PDZ3 Allosteric Communication  
A. Ali, A. Gulzar, S. Wolf, and G. Stock, *J. Phys. Chem. Lett.* 13, 9862 (2022).

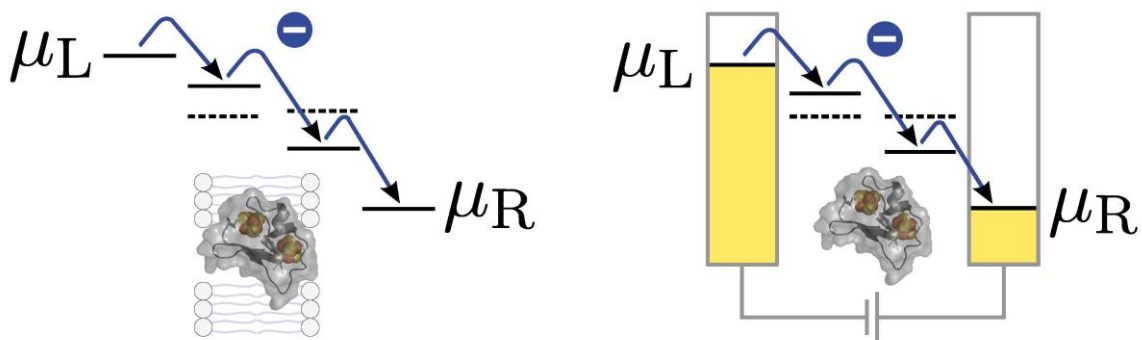
## High voltage rock'n'roll: a theoretical approach to protein electron transfer far from equilibrium.

Mike Castellano<sup>a</sup>, Christoph Kaspar<sup>b</sup>, Michael Thoss<sup>b</sup>, Thorsten Koslowski<sup>a</sup>

<sup>a</sup>Institute of Physical Chemistry, University of Freiburg, Albertstr. 21, 79104 Freiburg, Germany

<sup>b</sup>Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

Potential differences for protein-assisted electron transfer across lipid bilayers or in bio-nano setups can amount to several 100 mV (respiratory complex I, nitrite reductase, light-reduced processes), they lie far outside the range of linear response theory. We describe these situations by Kirchhoff-Master equations that are based on Marcus' theory of charge transfer between self-trapped electrons. In addition, we take on-site blockade effects and a full non-linear response of the local potentials into account. We provide analytical and numerical current-voltage curves and electron populations for multi-site model systems and biological electron transfer chains based on heme molecules or iron-sulfur clusters.



## Correlation-Based Feature Selection Unveils Functional Dynamics in Proteins

Gorg Diez and Gerhard Stock

Institute of Physics, University of Freiburg

Molecular dynamics simulations serve as a valuable tool to enhance our comprehension of proteins and their operational mechanisms. When analyzing these simulations, one often utilizes key internal coordinates to capture essential conformational changes since they are invariant under rotation and translation of the protein in its simulation box. Nonetheless, the interpretation is complicated by the resulting high-dimensional feature space, which contains both the crucial dynamics of the process of interest and subtle, intricate structural variations. These variations may not be pertinent to the functional dynamics and can consequently significantly impede the analysis.

To mitigate this complexity and enhance analysis, we introduce MoSAIC, an unsupervised, scalable feature selection approach that leverages correlations. MoSAIC effectively separates functional dynamics from noise, thus enabling a more comprehensive and insightful exploration of protein behaviors.

## **Log-periodic oscillations as result of hierarchical dynamics in proteins**

Emanuel Dorbath and Gerhard Stock

Institute of Physics, University of Freiburg

Processes of biomolecules exhibit motions on several timescales, ranging from fast vibrations (picoseconds) over local conformational changes (nanoseconds) to the global rearrangements (microseconds to seconds). These motions are seen as hierarchically coupled, where the fast vibrations are a prerequisite for the slower motions. This hierarchy can be understood by a one-dimensional free energy landscape which gives rise to a power law due to a discrete scale invariance. The scale invariance is also the reason for log-periodic oscillations seen in the time traces of molecular observables. The theoretical description of the discrete scale invariance and the emergence of log-periodic oscillations due to hierarchical dynamics are presented. Two systems are discussed: A one-dimensional model with four states separated by barriers of similar height is used as proof of principle. As second system, the peptide helix Aib9 is presented, which shows complex structural rearrangements. For both systems a time scale analysis is performed, a Markov State Model is generated, and a discrete scale invariance model is derived.

## Plasticity in amorphous carbon as a stress-assisted chemical reaction

Ibrahim Ghanem, Richard Jana, and Lars Pastewka

Amorphous carbon (a-C) films, due to their high wear resistance and excellent tribological properties, offer a remarkable solid lubricant for applications involving extreme mechanical conditions [1]. Since the lubrication process relies on the plastic flow of a-C films, it becomes essential to understand their plastic properties. We study the plasticity of a-C networks within the framework of shear transformation zones which are believed to be the fundamental carriers of plasticity in amorphous solids [2]. We use atomic-scale simulations to show that for amorphous carbon, a shear transformation can be reduced to a simple chemical reaction: the stress-induced breaking or forming of a single covalent bond. By forcing the breaking/forming of individual bonds in auxiliary calculations, we extract the potential energy landscapes of single bonds as a function of bond length. We find a good correlation between the energy barriers associated with a bond, the energy dissipated when the bond undergoes a plastic event, and the bond jump distance identified as the change in bond length due to the plastic event. Additionally, we apply a simple shear to an ensemble of a-C networks, all prepared by the same liquid-quench protocols, in the athermal quasistatic limit. By identifying plastic events that occur and using the correlation previously derived, we were able to calculate the average dissipated energy as a function of the applied strain. We use this to predict the yield stress of the carbon systems at hand. Our results help in interpreting some of the plastic properties of a-C networks and allow the parametrization of mesoscopic models of their plastic flow.

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## Active Responsive Colloids

Nils Göth

Institute of Physics, University of Freiburg

Dynamical polydispersity in single-particle properties, for example a fluctuating particle size, shape, charge density, etc, is intrinsic to responsive colloids (RCs), such as biomacromolecules or microgels, but is typically not resolved in coarse-grained mesoscale simulations.

Here, we present Brownian dynamics simulations of suspensions of RCs modeling soft hydrogel colloids, for which the size of the individual particles is an explicitly resolved (Gaussian) degree of freedom and dynamically responds to the local interacting environment. Furthermore, we introduce two model modifications to include activity in the system: On the one hand, a two-temperature model where the size degree of freedom is coupled to a thermostat with different temperature. On the other hand, a model where the size degree of freedom is driven by a dichotomous noise. We calculate for both cases the liquid structure, emergent size distributions and long-time diffusion. Our study indicates that particle dynamical polydispersity as well as the structure and dynamics of dense macromolecular suspensions can be vastly tuned by internal activity in terms of noise and internal “hot” or “cold” fluctuating states.

## **Nonadiabatic vibronic effects in single-molecule junctions: A theoretical study using the hierarchical equations of motion approach**

C. Kaspar<sup>1</sup>, A. Erpenbeck<sup>2</sup>, J. Bätge<sup>1</sup>, C. Schinabeck<sup>1</sup>, and M. Thoss<sup>1</sup>

<sup>1</sup>) Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3,  
D-79104 Freiburg, Germany

<sup>2</sup>) Department of Physics, University of Michigan, Ann Arbor, Michigan  
48109, USA

The coupling of electronic and nuclear degrees of freedom is an important mechanism in nonequilibrium charge transport in molecular junctions and may result in a variety of interesting phenomena such as decoherence, switching and local cooling or heating [1]. While the effect of adiabatic polaron-type coupling has been studied in great detail, new phenomena are expected for nonadiabatic coupling scenarios which correspond to a breakdown of the Born-Oppenheimer approximation. In this contribution, we present results of a model study of non-adiabatic effects employing the hierarchical equation of motion approach [2,3].

This method generalizes perturbative master equation methods by including higher-order contributions as well as non-Markovian memory and allows for the systematic convergence of results. In particular, we observe a quantum transport behavior strongly influenced by the interaction with the vibrational modes [4].

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## **Adsorption characteristics of novel star polymers as lubricant additives**

Lars Kruse, Kerstin Falk, Michael Moseler

MicroTribology Center  $\mu$ TC – Fraunhofer IWM

Towards more energy-efficient vehicles, machines and industrial plants, the reduction of friction losses in tribological systems can make a further, important contribution. The trend to reduce the viscosity of the lubricating oil leads - keeping other conditions unchanged - to a lower lubricant film thickness, which is associated with the risk of greater wear. This can be addressed by using low-friction, wear-resistant component coatings - or by using film-forming polymers in the lubricant.

A promising approach has been explored in a joint effort of atomistic simulation (Fraunhofer IWM), sophisticated polymer synthesis (Fraunhofer LBF) and lubricant development (Fuchs lubricants): Star polymers that do not noticeably thicken the lubricating oil, but are interfacially active.

This poster contribution focusses on the mode of action of these star polymer additives, namely their adsorption characteristics. Utilizing molecular dynamics simulations, the free energy of adsorption is computed via two methods: Steered molecular dynamics (SMD) and Thermodynamic integration (TI). By variation of the star polymer structure, structure-property relationships are investigated, to ultimately find an optimized star polymer molecule as lubricant additive.



## **Current-Induced Bond Rupture in Molecular Junctions: A Semi-Classical Langevin Approach Based on Electronic Friction**

Martin Mäck, Samuel Rudge, and Michael Thoss

Institute of Physics, University of Freiburg

<https://www.thcp.uni-freiburg.de/>

A common setup to investigate transport phenomena in open quantum systems is a molecular junction. Such devices consist of a molecule that is attached to two electrodes and driven out of equilibrium. The interaction between electronic and vibrational degrees of freedom can play an important role for electron transport in molecular junctions and is fundamental for current-induced bond rupture, which is a crucial aspect for their stability [1, 2]. However, accurate quantum mechanical simulations of the bond rupture dynamics are numerically expensive, which is why vibrations are often treated semi-classically as influenced by fully quantum mechanically treated electronic degrees of freedom.

In this contribution, we use the hierarchical equations of motion (HEOM) approach [3] to semi-classical Langevin dynamics [4] to simulate the bond rupture dynamics of a system with anharmonic nuclear potentials and a non-linear electron-vibrational coupling. Moreover, we recently extended our approach to incorporate systems with a position-dependent molecule-lead coupling to realistically describe the vibrational dynamics for displacements far from the equilibrium position. By directly comparing our results to full quantum-mechanical simulations, we explore regions of applicability of our approach.

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## **Benchmarking Markov State Models: A Case Study on the Folding of HP35**

Daniel Nagel and Gerhard Stock

Institute of Physics, University of Freiburg

Markov state models (MSMs) have emerged as a widely used method for characterizing molecular dynamics (MD) trajectories in terms of memoryless transitions between metastable conformational states. Using a 300 $\mu$ s-long MD trajectory of the reversible folding of the villin headpiece (HP35) published by D. E. Shaw Research, we construct an MSM of the folding process based on interresidue contacts that reproduces the MD folding times and predicts that both the native basin and the unfolded region of the free energy landscape are partitioned into multiple structurally well-defined and metastable substates. Recognizing the need to establish non-trivial benchmark problems, we investigate to what extent and in what sense this MSM can be used as a reference model. To this end, we test the robustness of the MSM by comparing it to models that use alternative combinations of features, dimensionality reduction methods, and clustering schemes.

## **Rigorous numerical method beyond the Markov, Born and perturbative approximations: simulations of gate sequences of qubits in presence of noise**

Kiyoto Nakamura

University of Ulm

To describe dissipative dynamics of qubits in a rigorous manner, a recently developed extended Free-Pole Hierarchical Equations of Motion (FP-HEOM) [M. Xu et al., Phys. Rev. Lett. 129, 230601 (2022)] is introduced. Dynamics of a single qubit coupled to a reservoir during pulse sequences are numerically studied. We examine memory effects of the reservoir during a pulse sequence and the performance of the dynamical decoupling under an influence of the reservoir. For the boson reservoir, Ohmic and sub-Ohmic spectral densities are adopted. Especially, we focus on the effects of sub-Ohmic reservoirs, considering that they correspond to  $1/f$ -type noises.

## Mean-field models for the chemical fueling of transient soft matter states

Sven Pattloch

Institute of Physics, University of Freiburg

The chemical fueling of transient states (CFTS) is a powerful process to control the nonequilibrium structuring and the homeostatic function of adaptive soft matter systems. Here, we introduce a simple mean-field model of CFTS based on the activation of metastable equilibrium states in a tilted 'Landau' bistable energy landscape along a coarse-grained reaction coordinate (or 'order parameter') triggered by a nonmonotonic two-step chemical fueling reaction. Evaluation of the model in the quasi-static (QS) limit - valid for fast system relaxation - allows us to extract useful analytical laws for the critical activation concentration and duration of the transient states in dependence of physical parameters, such as rate constants, fuel concentrations, and the system's distance to its equilibrium transition point. We apply our model in the QS limit explicitly to recent experiments of CFTS of collapsing responsive microgels and find a very good performance with only a few global and physically interpretable fitting parameters, which can be employed for programmable material design. Moreover, our model framework also allows a thermodynamic analysis of the energy and performed work in the system. Finally, we go beyond the QS limit, where the system's response is slow and retarded versus the chemical reaction, using an overdamped Smoluchowski approach. The latter demonstrates how internal system time scales can be used to tune the time-dependent behavior and programmed delay of the transient states in full nonequilibrium.

## **Witnessing non-Markovianity in quantum Brownian motion by quasi-probability distributions in phase-space**

Irene Ada Picatoste

Institute of Physics, University of Freiburg

The theory of open quantum systems aims to describe the dynamics of a quantum system coupled to an environment using a limited number of degrees of freedom. The Caldeira-Leggett model of quantum Brownian motion represents a physically interesting example of such systems showing strong memory effects, i.e., non-Markovian dynamics, in certain parameter regimes. Recently, a witness for non-Markovianity has been developed which is based on the Kolmogorov distance between quasi-probability distributions of two states [1]. Additionally, for Gaussian dynamics, a new measure of non-Markovianity can be defined using exclusively the Glauber-Sudarshan P-function. Here, we apply this witness to the Caldeira-Leggett model and show the behaviour of the non-Markovianity measure in different scenarios, while studying the parameter regions where the witness works best.

## Applications of Landauer's blowtorch effect in nonequilibrium transport through molecular junctions

Riley Preston and Daniel Kosov

Institute of Physics, University of Freiburg, Hermann-Herder-Strasse 3, 79104  
Freiburg, Germany

Rolf Landauer's formulation of the so-called "blowtorch theorem" in 1975 demonstrated that the relative stability of locally stable states in a potential depends not only on the energy landscape itself, but also the kinetics along the intervening states between points of stability [1]. Systems immersed in a non-equilibrium environment, in which the temperature across the potential is inhomogeneous, can then exhibit novel effects, including the enhanced relative stability of traditionally unstable states, and periodic motion through the potential.

Such effects emerge naturally in molecular junctions, where a molecular bridge is embedded in a far-from-equilibrium electronic environment via contact with two conducting leads. Electrons tunneling through the system produce current-induced forces which excite vibrations in nuclei along the molecular bridge. These vibrations can be quantified in terms of a local effective temperature, whose magnitude depends crucially on the geometry of the bridge. The relative stability of different molecular geometries may then be altered by a locally applied blowtorch (temperature spike) along the intervening states, as determined by the electronic properties of the bridge [2].

We model the collective vibrations of the molecular bridge in molecular junctions according to a semi-classical Langevin equation, whereby the current-induced forces acting on a classical reaction coordinate are calculated quantum mechanically via non-equilibrium Green's functions. Under this approach, the reaction coordinate evolves along a potential of mean force while under the influence of an inhomogeneous temperature, which arises due to the interplay between the excitational stochastic force, and the usually dissipative frictional force; both of which are dependent on the classical coordinate. We apply our theory to the catalysis of non-equilibrium chemical reactions in molecular junctions, where we observe the inhomogeneous temperature to play a vital role in determining chemical reaction rates [3]. Additionally, we consider a model system in which the blowtorch effect is utilised as an entirely novel method of driving the rotation of a nanoscale molecular motor [4].

### References

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## Nonequilibrium dynamics in spin valve heterojunctions

Rudolf Smorka<sup>1</sup>, Pavel Baláž,<sup>2</sup> Martin Žonda<sup>3</sup>, and Michael Thoss<sup>1</sup>

<sup>1</sup>Institute of Physics, Albert-Ludwigs-Universität Freiburg

<sup>2</sup>FZU - Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic

<sup>3</sup>Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

Manipulation of magnetization by electric currents enables novel functions for spin-transfer torque devices playing a pivotal role in various technological applications such as magnetic memory devices, spintronic logic elements, and magnetic sensors. Beyond their immediate technological significance, these devices also serve as model systems, providing insights into a multitude of fundamental questions surrounding spin relaxation, spin-transfer torques, and other nonequilibrium phenomena. In this study, we investigate a two dimensional spin valve heterojunction, composed of a ferromagnet/normal metal/ferromagnet device modeled using a classical spin Kondo lattice model and interconnected with source and drain electrodes. We employ a combination of mixed quantum-classical Ehrenfest approach and hierarchical equation of motion technique to explore voltage-driven nonequilibrium spin dynamics and spin-transfer torques in these systems. In an isolated valve for short spacer layers and weak spin-electron couplings, magnetization dynamics of the ferromagnetic layers is in agreement with the macrospin approximation. For large spacer layers, our quantum-classical approach predicts electron-induced spin relaxation. For intermediate electron-spin couplings, a change in the localization character of the electronic eigenstates from metallic-like to insulator-like leads to a reduced indirect exchange interaction between spins mediated by the conduction electrons. As we extend our study to spin valve coupled to leads, we observe that spin relaxation times differ by several orders of magnitude depending on whether the DC bias is introduced by shifting the electrochemical potentials of both leads symmetrically about the equilibrium Fermi level of the spin valve (reminiscent of a gate-tunable junction) or by shifting the chemical potential of only one lead (as realized in a scanning tunneling microscope geometry).

## **Shear thinning behavior of PAO4 with ZDDP additive in bulk liquid**

Franziska Stief, Thomas Reichenbach, Kerstin Falk, Michael Moseler

Fraunhofer Institute for Mechanics of Materials IWM  
Institute of Physics, University of Freiburg

In times of downsizing, lubricants experience often extreme conditions such as high shear rates and extreme pressures. Both can render base oils that are traditionally considered Newtonian lubricants into shear thinning liquids. Therefore, a detailed knowledge of a lubricant's shear thinning behavior is crucial for the choice of a lubricant for a specific application. The focus of this work is the base oil PAO4 as lubricant in combination with the additive Zinc dialkyl dithiophosphate (ZDDP). With molecular dynamics (MD) simulations, the rheological properties are investigated: For a variation of pressures and temperatures, pure PAO4, PAO4 with 0.5 wt% and 5 wt% of the ZDDP additive are simulated as bulk liquid where shear rates of five orders of magnitude are applied and the viscosities are calculated. Within the bulk liquid, the additive doesn't significantly impact the rheological properties. Using the Carreau equation for the individual fits of the shear thinning curves and the Roelands equation describing the Newtonian viscosities, a constitutive law for PAO4's shear thinning behavior is formulated attributing the viscosities to the macroscopic parameters of pressure and temperature. The observed shear thinning is rationalized by structural order parameters.



## Exploring Dry Friction of Amorphous Carbon on Epitaxial Graphene: Insights and Observations

Mohammad Zarshenas, Thomas Reichenbach, Gianpietro Moras and Michael Moseler

Fraunhofer Institute for Mechanics of Materials IWM  
Institute of Physics, University of Freiburg

In this study, we investigated the sliding behavior of H/OH-terminated amorphous carbon (a-C) on the graphene/SiC system at 300 K. The study is divided into two distinct phases. The initial phase involves the utilization of Density-Functional Tight-Binding (DFTB) simulations to explore friction regimes under varying pressures, encompassing both low (ranging from 5 to 15 GPa) and high (ranging from 17.5 to 30 GPa) conditions. In the subsequent phase, classical Molecular Dynamics (MD) simulations were conducted to scrutinize the super-low sliding regime, extending up to 100 nN (equivalent to 3.5 GPa), employing a non-reactive force field.

Our DFTB results show that, at low pressures (up to 15 GPa) during the 200 ps simulation, there are no reactions between a-C and the underlying graphene, resulting in smooth sliding behavior. Initially, the shearing plane is located between a-C and graphene. However, as pressure increases (from 17.5 GPa to 20 GPa), significant changes occur. Within the first 30 ps, the two graphene layers bond, and inner a-C atoms form bonds with graphene. As the simulation progresses, hydrogen atoms break bonds with a-C and form new ones with graphene, partially passivating it. This shift in behavior is reflected in the velocity gradient, transitioning from being situated between graphene layers to being between a-C and the graphene layer. At higher pressures (>30 GPa), graphene begins amorphizing within the first few picoseconds of the simulation.

Classical MD simulations are faster than DFTB simulations, allowing us to mimic experimental scales using a 20 nm a-C tip. Molecular statics precisely replicate slow tip movements, incrementally displaced in 0.2 Å steps for indentation and scratching. Simulations covered pressures from 20 nN to 100 nN (1.9 GPa to 3.3 GPa) with results based on 30 Å indentation. Findings for the H-terminated tip show a low friction force (ranging from 0.034 to 0.136 nN) that increases with applied pressure. Introducing an H/OH-terminated tip substantially increases friction force (ranging from 6.62 to 8.13 nN), which is proportional to the normal load. Notably, the friction forces consistently remain nonzero, diverging from experimental observations reporting zero friction within this pressure range. This emphasizes the significance of termination groups. Future simulations will explore oxygen-terminating groups like ether, aiming to achieve smoother sliding behavior and near-zero friction within experimental pressure ranges.

## List of Participants

### Invited Speakers

**Bocquet, Lydéric**

Centre national de la recherche scientifique – 3 Rue Michel Ange – Paris, France

**Carloni, Paolo**

Forschungszentrum Jülich GmbH – Wilhelm-Johnen-Straße – Jülich, Germany

**Dellago, Christoph**

University of Vienna – Computational and Soft Matter Physics – Kolingasse 14-16 – Vienna, Austria

**Huang, Xuhui**

University of Wisconsin-Madison – Department of Chemistry – 1101 University Avenue – Madison, USA

**Klapp, Sabine**

Technical University of Berlin – Eugene-Paul-Wigner-Gebäude Hardenbergstr. 36 – Berlin, Germany

**Kremer, Kurt**

Max-Planck-Institut für Polymerforschung – Ackermannweg 10 – Mainz, Germany

**Laio, Allesandro**

SISSA – Via Bonomea 265 – Trieste, Italy

**Makarov, Dimitrii E.**

Oden Institute – 201 E. 24<sup>th</sup>. St. – Austin Texas, USA

**Netz, Roland**

Freie Universität Berlin – Arnimallee 14 – Berlin, Germany

**Peter, Christine**

University of Konstanz – Department of Chemistry – Universitätsstrasse 10 – Konstanz, Germany

**Segal, Dvira**

University of Toronto – Department of Chemistry – 80 St. George Street – Toronto, Canada

**Seifert, Udo**

University of Stuttgart – Institute of Theoretical Physics – Pfaffenwaldring 57 – Stuttgart, Germany

**Speck, Thomas**

University of Mainz – Institute of Physics – Staudingerweg 9 – Mainz, Germany

**Strunz, Walter**

Technical University Dresden – Institute of Physics – Helmholtzstraße 10 – Dresden, Germany

**Tanimura, Yoshitaka**

Kyoto University – Department of Chemistry -

**Tiwary, Praytush**

University of Maryland – Department of Chemistry & Biochemistry – 8051 Regents Drive – College Park, US

### University Freiburg Pls

**Stock, Gerhard**

University of Freiburg – Institute of Physics – Hermann-Herder-Strasse 3a – Freiburg, Germany

**Thoss, Michael**

University of Freiburg – Institute of Physics – Hermann-Herder-Strasse 3a – Freiburg, Germany

**Breuer, Heinz-Peter**

University of Freiburg – Institute of Physics – Hermann-Herder-Strasse 3a – Freiburg, Germany

**Dzubiella, Joachim**

University of Freiburg – Institute of Physics - Hermann-Herder-Strasse 3 – Freiburg, Germany

**Falk, Kerstin**

Fraunhofer Institute for Mechanics of Materials IWM – Wöhlerstr. 11 – Freiburg, Germany

**Koslowski, Thorsten**

University of Freiburg – Institute of phys. Chemistry – Albertstr. 23a – Freiburg, Germany

**Moseler, Michael**

University of Freiburg – Institute of Physics & Fraunhofer Institute for Mechanics of Materials IWM – Wöhlerstr. 11 – Freiburg, Germany

**Pastewka, Lars**

University of Freiburg – Department of Microsystems Engineering– Georges-Köhler-Allee 103 – Freiburg, Germany

**Schilling, Tanja**

University of Freiburg – Institute of Physics - Hermann-Herder-Strasse 3 – Freiburg, Germany

**Wolf, Steffen**

University of Freiburg – Institute of Physics - Hermann-Herder-Strasse 3 – Freiburg, Germany

## Participants

**Ali, Ahmed**

University of Freiburg – Institute of Physics - Hermann-Herder-Strasse 3 – Freiburg, Germany

**Amati, Graziano**

University of Freiburg – Institute of Physics - Hermann-Herder-Strasse 3 – Freiburg, Germany

**Castellano, Mike**

University of Freiburg – Institute of phys. Chemistry – Albertstr. 23a – Freiburg, Germany

**Cortes-Huerta, Robinson**

Max-Planck-Institut für Polymerforschung– Ackermannweg 10 – Mainz, Germany

**Diez, Georg**

University of Freiburg – Institute of Physics - Hermann-Herder-Strasse 3 – Freiburg, Germany

**Dorbath, Emanuel**

University of Freiburg – Institute of Physics - Hermann-Herder-Strasse 3 – Freiburg, Germany

**Ghanem, Ibrahim**

University of Freiburg – Department of Microsystems Engineering– Georges-Köhler-Allee 103 – Freiburg, Germany

**Göth, Nils**

University of Freiburg – Institute of Physics - Hermann-Herder-Strasse 3 – Freiburg, Germany

**Jäger, Miriam**

University of Freiburg – Institute of Physics - Hermann-Herder-Strasse 3 – Freiburg, Germany

**Kaspar, Christoph**

University of Freiburg – Institute of Physics – Hermann-Herder-Strasse 3a – Freiburg, Germany

**Kruse, Lars**

Fraunhofer Institute for Mechanics of Materials IWM – Wöhlerstr. 11 – Freiburg, Germany

**Mäck, Martin**

University of Freiburg – Institute of Physics – Hermann-Herder-Strasse 3a – Freiburg, Germany

**Milster, Sebastian**

University of Freiburg – Institute of Physics - Hermann-Herder-Strasse 3 – Freiburg, Germany

**Nagel, Daniel**

University of Freiburg – Institute of Physics - Hermann-Herder-Strasse 3 – Freiburg, Germany

**Nakamura, Kiyoto**

University of Ulm, Institute for Complex Quantum Systems, Albert-Einstein-Allee 11, 89069 Ulm, Germany

**Pattloch, Sven**

University of Freiburg – Institute of Physics - Hermann-Herder-Strasse 3 – Freiburg, Germany

**Picatoste, Irene Ada**

University of Freiburg – Institute of Physics – Hermann-Herder-Strasse 3a – Freiburg, Germany

**Preston, Riley**

University of Freiburg – Institute of Physics – Hermann-Herder-Strasse 3a – Freiburg, Germany

**Richter, Moritz F.**

University of Freiburg – Institute of Physics – Hermann-Herder-Strasse 3a – Freiburg, Germany

**Rudge, Samuel**

University of Freiburg – Institute of Physics – Hermann-Herder-Strasse 3a – Freiburg, Germany

**Sartore, Sofia**

University of Freiburg – Institute of Physics – Hermann-Herder-Strasse 3a – Freiburg, Germany

**Smorka, Rudolf**

University of Freiburg – Institute of Physics – Hermann-Herder-Strasse 3a – Freiburg, Germany

**Stief, Franziska**

Fraunhofer Institute for Mechanics of Materials IWM – Wöhlerstr. 11 – Freiburg, Germany

**Zarshenas, Mohammad**

University of Freiburg – Institute of Physics & Fraunhofer Institute for Mechanics of Materials IWM – Wöhlerstr. 11 – Freiburg, Germany

RU Workshop - Programme

	Tuesday, 19.09.2023	Wednesday, 20.09.2023	Thursday, 21.09.2023	Friday, 22.09.2023
08:45	Welcome			
09:00	Tiwary	Tanimura	Huang	Kremer
09:40	Dellago	Rudge	Peter	Klapp
10:20	Milster	Segal	Stock	Falk
11:00	Coffee Break	Coffee Break	Coffee Break	Coffee Break
11:30	Seifert	Strunz	Laio	Makarov
12:10	Sartore	Richter	Koslowski	Closing
12:30	Jäger			
13:00		Amati		
	Lunch Break		Lunch Break	
14:00	Bocquet		Carloni	
14:40	Moseler	Netz	Wolf	
15:20	Pastewka	Schilling	Coffee Break	
16:00	Coffee Break	Speck	Excursion & Dinner	
16:30	Postersession	Coffee Break		
		Free evening		
18:30	Free evening			