Public Presentation at the Faculty of Physics Date: 25 September 2019
Place: Ernst-Mach lecture hall, 2nd floor, Boltzmanngasse 5, 1090 Wien

Time Slot	Name	Topic	Supervisor
9:00-9:10	--	Introduction by Markus Arndt (in representation of Thomas Pichler)	
9:10-9:25	Ventura Rosales Ivonne Elizabeth	Coarse-graining and self-assembly of associating polymer in confined geometry	Christos Likos
9:25-9:40	Kaiser Martin	Directing dipolar active Matter with applied fields	Sophia Kantorovic
9:40-9:55	Pitters Johanna	Methods for Accelerator Mass Spectrometry (AMS) of 99 Technetium	Robin Golser Karin Hain
9:55-10:10	van Valkenhoef Céline Hélène Ida	Quantum information processing in the human brain	Philip Walther
10:10-10:40	**Jonathan Lahnsteiner**	**Phase transitions of hybrid perovskites simulated by machine-learning force fields**	
10:40-11:10	COFFEE BREAK		
11:10-11:25	Ananda Wisnu	Structural properties and electric behavior of CZTS solar cells and devices	Wolfgang Lang
11:25-11:40	Kull Ilya	Spacetime area laws for quantum information	Caslav Brukner
11:40-11:55	Lechner Daniel	Electroweak Effects in Top Quark Pair Production and Top Quark Mass Determinations in the Boosted Framework	André Hoang
11:55-12:10	Lüdke Jan	Short-distance constraints on the hadronic light-by-light contribution to the muon g-2	Massimiliano Procura
12:10-12:40	**Paulus Bauer**	**In-situ Aerosol Nanoparticle Characterization by Small Angle X-ray Scattering (SAXS)**	
12:40-13:40	LUNCH BREAK		
13:40-13:55	Pseiner Johannes	Novel Long Distance Free Space Quantum Coherence and Quantum Key Distribution Experiments	Anton Zeilinger
13:55-14:10	Trentino Alberto	Defect engineering in 2D-Materials by Ions beams irradiation	Jani Kotakoski
14:10-14:25	Reisz Niklas	Statistical mechanics based approach to understanding information flow process in complex systems	Stefan Thurner Christoph Dellago
14:25-14:40	Vyvlecka Michal	Cluster State Quantum Computing using Solid-State Photon Sources	Philip Walther
14:40-15:10	**Irati Alonso Calafell**	**Quantum Computing with Graphene Plasmons**	
15:10-15:30	COFFEE BREAK		
15:30-15:45	Widl Angelika	Top Quark Pair Production at Future Lepton Collidiers: Differential Cross Section from Threshod to Continuum at NLL/NLO	André Hoang
15:45-16:00	Knopik Jerzy	Geometric Properties of Black Holes	Piotr Chrusciel
16:00-16:15	Hahn Thomas	Electron-Photon Coupling: From First Principles to Model Hamiltonians	Cesare Franchini
16:15-16:30	Conrad-Billroth Clara	Enhancing Interferometric Microscopy Techniques using self-imaging Cavities	Thomas Juffmann
16:30-16:45	Ivetic Boris	Geometry of energy-momentum manifold and Poincare symmetry	Stefan Fredenhagen Salvatore Mignemi

Phase transitions of hybrid perovskites simulated by machine-learning force fields[1]

Jonathan Lahnsteiner

[1] R. Jinnouchi, J. Lahnsteiner, F. Karsai, G. Kresse and M. Bokdam Phys. Rev. Lett. 122, 225701 (2019)

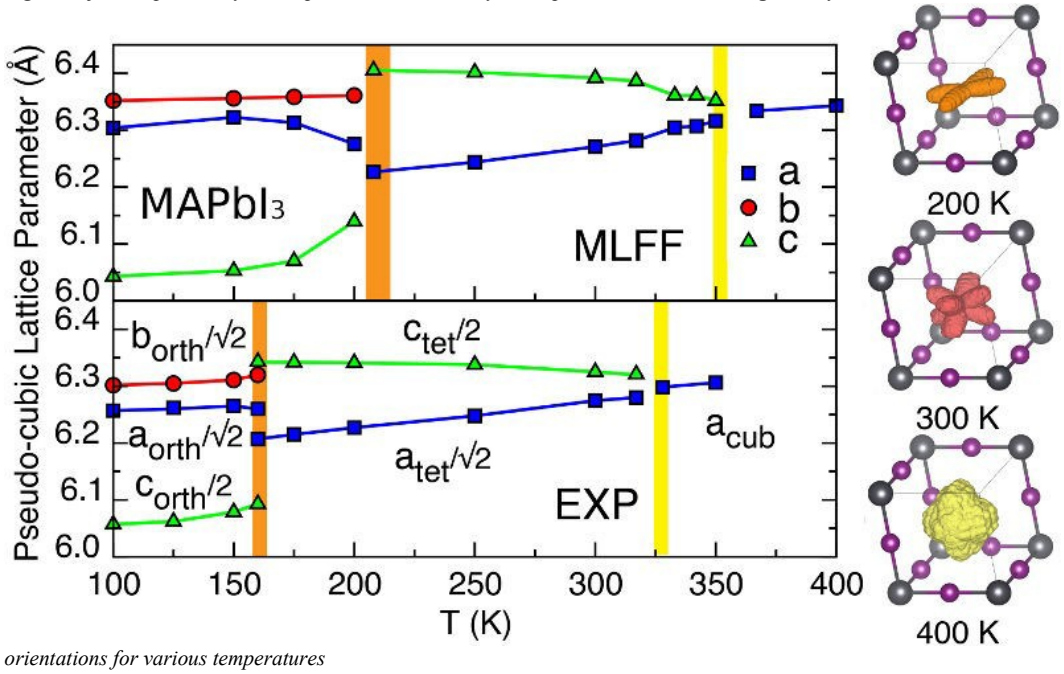
Abstract

Realistic finite temperature simulations of matter are a formidable challenge for first principles (FP) methods. Long simulation times and large length scales are required, demanding years of compute time. Here we present an on-the-fly machine learning scheme that generates force fields automatically during FP based molecular dynamics (MD) simulations. This opens up the required time and length scales, while retaining the distinctive chemical precision of FP methods. The method is widely applicable to multi-element complex systems. In this talk, the power of the scheme is demonstrated by applying it to the entropy driven phase transitions of hybrid perovskites.

The first part of the talk highlights how limited our atomistic understanding of the structure of $MAPbI_3$ is despite numerous FP studies. One of the problems is that depending on the employed density functional, very different predictions for the structure of $MAPbI_3$ are obtained. The question which functional is "right", is not easily addressed by comparison with experiment [2]. Here, we use the strategy to generate ensembles using the random phase approximation to the correlation energy and compare the variance between RPA and DFT total energies. This allows us to choose the "best" functional from a pool of considered functionals [3].

In the second part of the talk the "best" functional (SCAN) is used to train a machine -learning force field (MLFF) of $MAPbI_3$ on-the-fly during MD calculations [1]. The machine examines possible errors in the MLFF and automatically assesses the need for FP calculations. In this way, more than 99 % of the expensive FP calculations are bypassed, and MD simulations are accelerated by more than two orders of magnitude. Using machine learned potentials, isothermal-isobaric simulations give direct insight into the underlying microscopic mechanisms. We show how the phase transitions proceed on the nanosecond time scale, and we determine the order of the transitions in Landau theory. Finally, we relate the predicted phase transition temperatures of different inorganic perovskites to the radii of the involved species.

Fig. 1: ***Left:*** *Comparison of lattice parameters obtained from experiment and MLFF.* ***Right:*** *Preferred molecular orientations for various temperatures*



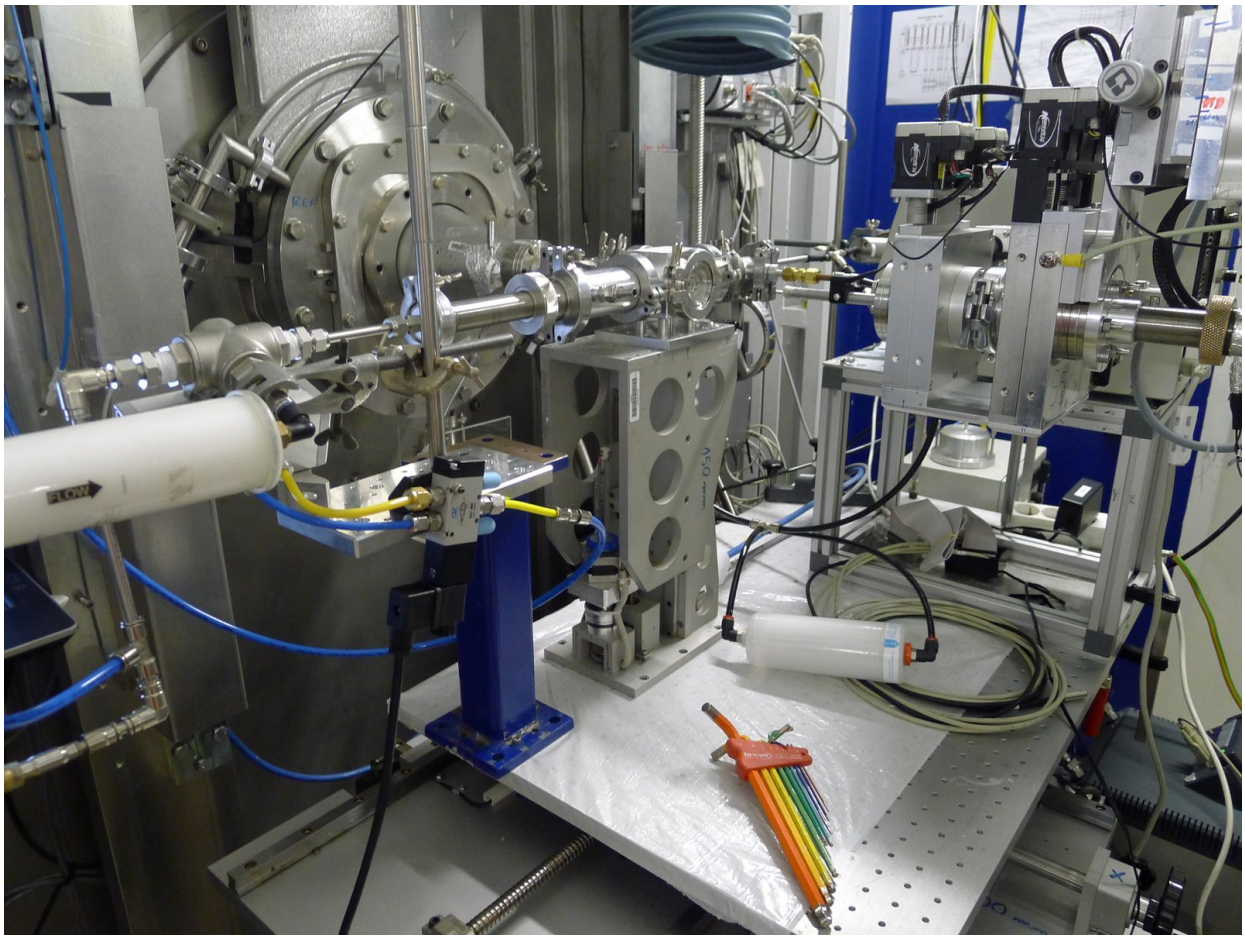
[2] J. Lahnsteiner, G. Kresse, J. Heijnen and M. Bokdam, Phys. Rev. Mat., 2, 073604 (2018)
[3] M. Bokdam, J. Lahnsteiner, B. Ramberger, T. Schäfer, and G. Kresse, Phys. Rev. Lett. 119, 145501 (2017)

In-situ Aerosol Nanoparticle Characterization by Small Angle X-ray Scattering (SAXS)

Dr. Paulus Bauer

Abstract

State-of-the-art aerosol nanoparticle techniques all have one feature in common: for analysis they remove the nanoparticles from their original environment. Therefore, physical and chemical properties of the particles might be changed or cannot be measured correctly. To overcome these shortcomings, synchrotron based small angle X-ray scattering (SAXS) was applied as an in-situ measurement technique. Contrasting other aerosol studies utilizing SAXS, comparatively low particle concentrations are used in this study which allows parallel measurements with conventional aerosol analyzers. To this end, tungsten and silver nanoparticles are measured at ambient pressure and concentrations of about 10^6 cm^{-3}. Air and helium are used as carrier gas. The latter one reduces the scattering background of the carrier gas up to one order of magnitude compared to air. A conventional differential mobility particle sizer (DMPS) and condensation particle counter (CPC) are operated in air and helium and measure the size distribution and concentration in parallel. The findings are complemented by TEM images taken from the nanoparticles. By this comprehensive combination of the various techniques measurements of the concentration, size and morphology of the aggregates and primary particles are possible. The acquired data thus enables profound insights on the formation process of the nanoparticles. To conclude, in-situ nanoparticle characterization with ultra-low volume fractions of 10^{-10} is feasible with SAXS providing important information on the morphology and hence on the formation process of the nanoparticles.



Quantum Computing with Graphene Plasmons

I. Alonso Calafell[1], Joel D. Cox[2], Milan Radonjic[1], J. R. M. Saavedra[2], Javier García de Abajo[2,3], Lee A. Rozema[1] and Philip Walther[1]

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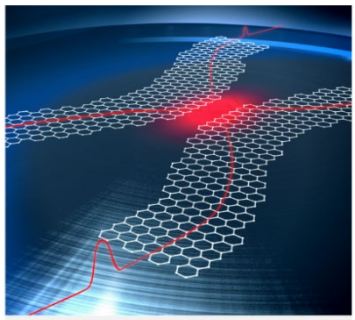
Photons, the smallest particles of light, are also the fastest and barely interact with the environment, being able to travel vast distances without flinching at all. Although these features make these little particles one of the most promising candidates for quantum communication applications, these features also make them especially difficult to manipulate and handle. In photonic quantum computing, information is encoded in photons and these are mixed together in different ways depending on the computation that one wants to perform, and the final state of the photons contains the result of this computation.

Due to the weak interaction of the photons with their environment, these mixing processes known as nonlinear interactions do not naturally occur in the air and one needs to send the photons to a so called nonlinear material to make the photons interact with each other. Nowadays, there are many nonlinear materials available but they are all extremely inefficient, making it impossible to carry out large computations with many photons. In other words, current nonlinear materials allow us having quantum calculations but prevent us from building a powerful quantum computer.



Schematic of a graphene-based two-photon gate

This new proposed platform for quantum computation takes advantage of the strong nonlinear properties of graphene. This 2D material discovered barely a decade ago consists of a single layer of carbon atoms arranged in a honeycomb structure and its characteristics do not stop surprising us. For this particular purpose, the peculiar configuration of the electrons in graphene leads to an extremely strong nonlinear behavior that boost the efficiency of such nonlinear interactions to unprecedented values.

In this newly proposed scheme, photons are sent through a graphene nanoribbon, where the energy of the photon creates an electronic wave with similar characteristics as the photon that created it. These waves are known as plasmons and their behavior in these sort of materials is comparable to the behavior of photons in the air, with the remarkable exception that plasmons strongly interact with each other.