Fachbereich Physik

GOETHE UNIVERSITÄT FRANKFURT AM MAIN

Vorträge im Physikalischen Kolloquium

Sommersemester 2022

Mittwochs 16 Uhr c.t., Hörsaal _.111 (EG), Max-von-Laue-Str. 1

04.05.2022 **Dr. Jürgen Köfinger** (Max-Planck-Institut für Biophysik, Goethe-Universität Frankfurt) - Habilitation-Antrittsvorlesung

Integration of experimental data and molecular simulations

To understand life on the molecular level, we apply molecular dynamics simulations to increasingly larger and more complex biomolecular systems over longer times. We aim to maximize the predictive power of these simulations by choosing an appropriate molecular model or force field to trade off sampling errors and systematic force field errors. We further alleviate these intrinsic limitations by integrating additional experimental information. After introducing some basic concepts, capabilities, and goals of biomolecular simulations, I will discuss the use of Bayes theorem to refine molecular simulations by integrating ensemble averaged experimental data. The Bayesian inference of ensembles (BioEn) method [Hummer and Köfinger, J. Chem. Phys. (2015)] preserves the character of the simulation ensemble while it improves the agreement with the data. The resulting refined ensemble is a better representation of the true ensemble underlying the data. On this basis, I will introduce the Bayesian inference of force fields (BioFF) method [Köfinger and Hummer, N. J. Phys. B (2021)] to refine force field parameters using various data. BioFF systematically resolves force field issues and encodes learned information directly in the force field. These refined force fields are transferable and can

be applied to diverse biomolecular systems. Such formalized, systematic, and (semi)automatic machine-learning efforts to ensemble refinement and force field optimization are set to play an indispensable role in the promising future of biomolecular simulations.

local host: Dekan Prof. Dr. Harald Appelshäuser | appels@ikf.uni-frankfurt.de

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18.05.2022 **Prof. Dr. John Briggs** (Universität Freiburg)

Time in Quantum Mechanics

As a long-time practitioner of quantum theory I venture to question the commonlyheld view that the Time-Dependent Schroedinger Equation (TDSE) is the fundamental quantum equation from which the Time-Independent Schroedinger Equation (TISE) is obtained as a special case. I advance arguments to show that rather it is the TDSE which should be viewed as a half-classical approximation to the TISE, where one variable emerges as classical time. I begin with an overview of Schroedinger's route to the TDSE in 1926. The argument is supported by parallel demonstrations of the emergence of time in classical mechanics, in paraxial optics and in quantum gravity. The talk is perhaps relevant particularly to physics students.

local host: Prof. Dr. Reinhard Dörner | doerner@atom.uni-frankfurt.de

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25.05.2022 Apl-Prof. Dr. Giuliano Franchetti (Institut für Angewandte Physik, Goethe-Universität Frankfurt) - Antrittsvorlesung zur Verleihung der Apl-Professur

Frontiers in Accelerator & Beam Physics

The invention of particle accelerators has been instrumental to physics discoveries: the art of delivering more energetic and more intense particle beams has been symbiotic with the request of particle physics demands. This effort, over the course of the years, not only has provided new tools for discovery but has also made accelerator and beam physics emerge as a stand-alone discipline. This presentation will review the accelerator and beam physics challenges and their impact on present and future projects. The ongoing trend of pushing the accelerators frontier will be discussed as well.

local host: Prof. Dr. Holger Podlech | H.Podlech@iap.uni-frankfurt.de

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01.06.2022 Prof. Dr. Jorge Noronha (University of Illinois, USA)

Relativistic Fluid Dynamics: From Particle Colliders to Neutron Star Mergers

Heavy-ion collision experiments have provided overwhelming evidence that quarks and gluons, the elementary particles within protons and neutrons, can flow as a nearly frictionless, strongly interacting relativistic liquid over distance scales not much larger than the size of a proton. On the other hand, with the dawn of the multi-messenger astronomy era marked by the detection of a binary neutron star merger, it became imperative to understand how extremely dense fluids behave under very strong gravitational fields. Therefore, three of the most cutting-edge experimental apparatus in modern science, the Relativistic Heavy Ion Collider (RHIC), the Large Hadron Collider (LHC), and the Laser Interferometer Gravitational-Wave Observatory (LIGO) are now taking data whose description requires a major overhaul of our current understanding of fluid dynamics. In this talk I will discuss the new developments that have contributed to redefine the onset of relativistic fluid dynamics and its extension towards the far-from-equilibrium regime. New results involving viscous fluids and their coupling to general relativity will also be presented. These results pave the way for the inclusion of viscous effects in neutron star merger simulations.

local host: Prof. Dr. Dirk Rischke | drischke@itp.uni-frankfurt.de

15.06.2022 **PD Dr. Sven Barth** (Physikalisches Institut, Goethe-Universität Frankfurt)

Synthese anorganischer Nanomaterialien jenseits des thermodynamischen Gleichgewichts

The synthesis of nanomaterials and especially the molecule-to-material conversion under non-equilibrium conditions is dependent on precursors used for their formation. The lecture will focus on gas-phase growth techniques for the synthesis of inorganic nanomaterials and discuss the aspects of precursor selection for focused electron beam deposition (FEBID) as well as the formation of Ge-based nanomaterials of metastable composition.

In this respect, the growth of single crystalline Ge-based nanomaterials with metastable composition will be discussed and the overall impact of microstructure/composition on their physical properties shall be highlighted.

In addition, new precursors for FEBID techniques, which is an approach for direct writing of nanostructures, have been introduced and significant improvements in the understanding of fragmentation processes in the electron-induced fragmentation process have been gained. The fragmentation process leading to an inorganic deposit can be explained from a chemical point of view using model reactions and comparison to actual FEBID deposits' composition. Some features will be discussed on selected examples from our recent investigations.

local host: Prof. Dr. Jens Müller | j.mueller@physik.uni-frankfurt.de

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29.06.2022 **Wagemann** (Dechema) - AUSGEFALLEN

Die Rolle des Wasserstoffs für ein klimaneutrales Deutschland im Jahr 2045

local host: Prof. Dr. Horst Schmidt-Böcking | schmidtb@atom.uni-frankfurt.de

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13.07.2022 **Dr. Hendrik Hähnel** (Institut für Angewandte Physik, Goethe-Universität Frankfurt)

Status and Perspectives of the FRANZ Accelerator

The Frankfurt Neutron Source (FRANZ) is a compact accelerator driven facility originally initiated in the early 2000s. It is designed to provide a 2 MeV proton beam for neutron production via the 7Li(p, n)7Be reaction. The produced neutrons with a thermal spectrum around 30 keV can be used for a number of experiments in the fields of applied physics and experimental astrophysics.

Significant progress on the driver linac was made recently. The commissioning of the new CHORDIS ion source in late 2020 was a first milestone. Since the CHORDIS ion source only provides a 35 keV proton beam, an electrostatic post-accelerator was developed and commissioned at IAP to reach the desired beam energy of 60 keV. After stable operation was confirmed, the Low Energy Beam Line (LEBT) was commissioned and the beam was transported up to the point of Injection into the RFQ-Accelerator. This presents an important milestone for the initial beam commissioning of the FRANZ facility. The 2 MeV RF linac is presently being modified in one component to match the achieved beam conditions at injection. Meanwhile, emittance measurements to further improve an efficient injection into the RFQ are well under way.

I will present the recent progress since ca. 2019 and show a path to operation for first experiments with neutrons within the next two years. A new compressor concept for the production of short brilliant neutron bunches in the future will be shown as well.

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