TT 14: Artificial Intelligence in Condensed Matter Physics II (joint session TT/DY)

While artificial intelligence leaves an ever growing footprint in our everyday lives, it has as well inspired various new approaches in the physical sciences; for instance, one of the outstanding success stories is the prediction of protein folding with unprecedented accuracy. But what role can AI play in condensed matter physics? This symposium aims to provide an overview and discussion of recent applications of modern machine learning and its prospects for the advancement of research in this field. The increasingly data-intensive experiments with high-dimensional observations call for the development of new tools for analysis matching known strengths of machine learning algorithms. Reinforcement learning agents can be employed to precisely manipulate many-body systems, which, among other use cases, is a pivotal ingredient for quantum technologies. On the computational side, ideas from deep learning and generative modeling inspire new building blocks to boost numerical simulations. One may even ask the question whether a machine can autonomously discover physical concepts such as effective degrees of freedom or equations of motion, and reveal them in an interpretable manner to human researchers.

Prof. Dr. Simon Trebst, Universität Köln
Prof. Dr. Florian Marquardt, Max-Planck-Institut Erlangen
Dr. Markus Schmitt, FZ Jülich

Time: Monday 15:00–16:00 Location: H 3025

TT 14.1 Mon 15:00 H 3025

Uncertainty-aware active learning for interatomic potentials generation and its applications for spin dynamics — •Valerio Briganti and Alessandro Lunghi — School of Physics, AMBER and CRANN Institute, Trinity College, Dublin 2, Ireland

In the last decade, the materials science community has increasingly exploited the potential of AI for various applications, ranging from the discovery of new materials to the generation of interatomic potentials (IP). Developments in the latter have enabled to perform molecular dynamics simulations with unprecedented timescales, with the promise of successfully overcoming the computational costs required by ab initio methods keeping a sufficiently high accuracy. Two of the main challenges in this field are the design of models to allow greater transferability and the optimal selection of data to be included in the training set. In this contribution, I will show how a linear regression model based on SNAP [1] augmented with an uncertainty aware active learning procedure [2] can efficiently lead to the generation of accurate IPs able to simulate the dynamics of organic and open-shell compounds at room temperature. In addition to this, I will also present the performance of machine learning IPs for prediction of phonons and spin-phonon relaxation time.

[1] A.P. Thompson et al., J. of Comp. Phys., 285 (2015) 316.
[2] V. Briganti, A. Lunghi, Mach. Learn.: Sci. Technol. 4 (2023) 035005.

TT 14.2 Mon 15:15 H 3025

Transverse barrier and filament formation by electrical triggering of a metal-to-insulator or insulator-to-metal transition — •Lorenzo Fratino[1], Marcelo Rozenberg[2], Pavel Salev[3], Javier Del Valle[4], and Ivan K. Schuller[5] — [1]LPTM, CY Cergy Paris Université, Cergy-Pontoise — [2]LPS, Université Paris Saclay, Orsay — [3]University of Denver, USA — [4]University of Geneva, Switzerland — [5]University of California, San Diego, USA

By doing numerical simulations on Mott resistors network model, we were able to give a theoretical background to experimental observations on magnetotransport in ferromagnetic oxide (La,Sr)MnO_3 (LSMO) during electrical triggering of the intrinsic metal-insulator transition (MIT), which produces volatile resistive switching. This switching occurs in a characteristic spatial pattern, the formation of a paramagnetic insulating barrier perpendicular to the current flow, in contrast to the conventional filamentary percolation parallel to the current. This formation was also simulated in order to demonstrate that this process is triggered by nucleation at hotspots, with a subsequent expansion over several decades in time. By comparing three case studies (VO_2, V_3O_5, and V_2O_3), we identified the resistivity change across the transition as the crucial parameter governing this process. Our results provide a spatio-temporal characterisation of volatile resistive switching in Mott insulators, which is important for emerging technologies, such as optoelectronics and neuromorphic computing.

[1] Phys. Rev. B 108 (2023) 174434.
[2] Nat. Comm. 12 (2021) 1.
[3] Science 373 (2021) 907.

TT 14.3 Mon 15:30 H 3025

Autonomous bromine removal in scanning tunneling microscope — •Nian Wu[1], Markus Aapro[1], Alexander Ilin[2], Robert Drost[1], Joakim Jestilä[1], Zhijie He[2], Peter Liljeroth[1], and Adam S. Foster[1,3] — [1]Applied Physics, Aalto University, Helsinki, Finland — [2]Computer Science, Aalto University, Helsinki, Finland — [3]WPI Nano Life Science Institute, Kanazawa University, Kanazawa, Japan

More recent studies have even harnessed scanning probe microscopy (SPM) to control chemical reactions in on-surface molecular synthesis. In general, the SPM manipulations are predominantly controlled via parameters of the tip position, pulse voltages and tunneling conductance in scanning tunneling microscope (STM). However, the selection of proper parameters requires extensive domain knowledge, which is time-consuming and not necessarily transferable to new systems. Recent research has allowed the automation of a wide range of challenges, including lateral and vertical manipulation. However, the automation for breaking or forming covalent bonds, which is an indispensable step in chemical synthesis, is unexplored yet. To address this problem, we build on our deep reinforcement learning approach to automate the bromine removal from 5,15-bis(4-bromo-2,6-methyl-phenyl)porphyrin (Br_2Me_4DPP) through learning manipulation parameters in STM.

TT 14.4 Mon 15:45 H 3025

Neural quantum states for a two-leg Bose-Hubbard ladder under a magnetic field — •Kadir Çeven[1,2], Mehmet Özgür Oktel[2], and Ahmet Keleş[3] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany — [2]Department of Physics, Bilkent University, Ankara, Turkey — [3]Department of Physics, Middle East Technical University, Ankara, Turkey

This work explores novel quantum phases in a two-leg Bose-Hubbard ladder, achieved using neural quantum states. The remarkable potential of quantum gas systems for analog quantum simulation of strongly correlated quantum matter is well-known; however, it is equally evident that new theoretical bases are urgently required to comprehend their intricacies fully. While simple one-dimensional models have served as valuable test cases, ladder models naturally emerge as the next step, enabling studying higher dimensional effects, including gauge fields. Using [Çeven et al., PRA 106, 063320 (2022)], this work investigates the application of neural quantum states to a two-leg Bose-Hubbard ladder in the presence of strong synthetic magnetic fields. This paper showcased the reliability of variational neural networks, such as restricted Boltzmann machines and feedforward neural networks, in accurately predicting the phase diagram exhibiting superfluid-Mott insulator phase transition under strong interaction. Moreover, the neural networks successfully identified other intriguing many-body phases in the weakly interacting regime. These exciting findings firmly designate a two-leg Bose-Hubbard ladder with magnetic flux as an ideal testbed for advancing the field of neural quantum states.