Symposium Machine Learning in Atomic and Molecular Physics (SYML)

jointly organised by
the Molecular Physics Division (MO) and
the Atomic Physics Division (A)

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Machine-learning tools are increasingly employed to assist challenging problems in natural sciences. In atomic and molecular physics this notably includes the solution of the electronic Schrödinger equation, efficient quantum state tomography, problems in quantum computing and quantum simulation, optimal control of atomic systems, and inverse problems in x-ray-diffraction imaging and spectroscopy. This symposium gathers experts from experiments and theory and aims to provide an overview of this rapidly growing topic.

Overview of Invited Talks and Sessions

(Lecture hall E415)

Invited Talks

SYML 1.1	Tue	11:00–11:30	E415	**Imaging a complex molecular structure with laser-induced electron diffraction and machine learning** — •Katharina Chirvi, Xinyao Liu, Kasra Amini, Aurelien Sanchez, Blanca Belsa, Tobias Steinle, Jens Biegert
SYML 1.2	Tue	11:30–12:00	E415	**Physics-inspired learning algorithms for optimal shaping of atoms with light** — •Maximilian Prüfer
SYML 1.3	Tue	12:00–12:30	E415	**Machine-Learning assisted quantum computing and interferometry** — •Ludwig Mathey, Lukas Broers, Nicolas Heimann
SYML 1.4	Tue	12:30–13:00	E415	**Efficient quantum state tomography with convolutional neural networks** — •Moritz Reh, Tobias Schmale, Martin Gärttner

Sessions

SYML 1.1–1.4	Tue	11:00–13:00	E415	**Machine Learning in Atomic and Molecular Physics**

SYML 1: Machine Learning in Atomic and Molecular Physics

Time: Tuesday 11:00–13:00 Location: E415

Invited Talk SYML 1.1 Tue 11:00 E415

Imaging a complex molecular structure with laser-induced electron diffraction and machine learning — •Katharina Chirvi[1], Xinyao Liu[1], Kasra Amini[1], Aurelien Sanchez[1], Blanca Belsa[1], Tobias Steinle[1], and Jens Biegert[1,2] — [1]ICFO - Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels (Barcelona), Spain — [2]ICREA, Pg. Lluis Companys 23, 08010 Barcelona, Spain

Imaging a molecular structure with electron or X-ray diffraction relies on finding a global extremum in a multi-dimensional solution space. Laser-induced electron diffraction (LIED) is a powerful laser-based method that image the structure of a single gas-phase molecule with combined sub-atomic picometre and atto-to-femtosecond spatio-temporal resolution. In LIED, the structural information of the molecule is extracted from the coherently scattered electron wave packet, driven by an intense laser field after photoionization. However, retrieving the molecular geometry from a diffraction pattern becomes progressively difficult with increasing molecular structure and is a general challenge for any diffraction-based imaging technique. A machine learning (ML)-based approach is tailored to overcome this limitation since it achieves pattern matching in a complex solution space with high precision. We demonstrate the accurate retrieval of the three-dimensional structure of the chiral molecule Fenchone ($C_{10}H_{16}O$) by implementing LIED in combination with an ML algorithm. Our results show that ML-LIED provides new opportunities to determine the structure of large and complex molecules.

Invited Talk SYML 1.2 Tue 11:30 E415

Physics-inspired learning algorithms for optimal shaping of atoms with light — •Maximilian Prüfer — Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien

Nowadays the high degree of control over optical potentials is key to many quantum simulations performed with ultracold atomic systems. In this talk I will show how arbitrary optical potentials can be created using, e.g., digital micromirror devices. Experimentally it is advantageous to optimize the desired potentials 'offline', that is not using the actual experiment but a digital twin trained using machine learning methods. In our new approach we use a physics-inspired model with few parameters combined with an iterative algorithm based on Iterative Learning Control. These methods allow for model-based 'offline' optimization as well as experimental feedback-based 'online' optimization which leads to an order of magnitude faster optimization compared to heuristic methods.

Invited Talk SYML 1.3 Tue 12:00 E415

Machine-Learning assisted quantum computing and interferometry — •Ludwig Mathey[1,2], Lukas Broers[1], and Nicolas Heimann[1,2] — [1]Zentrum für Optische Quantentechnologien and Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

In this talk I will discuss our recent work on developing machine-learning based algorithms to control the complexity of technologies such as quantum computing and high-precision interferometry.

In the context of quantum machine learning, I will first discuss our work on mitigating barren plateaus. Barren plateaus present a challenge to efficient quantum machine learning which derives from vanishing gradients of the objective function. We point out that parametrizations that are non-local in time, such as a Fourier mode representation of the parameter space, can noticeably improve the performance. As a second objective in the context of quantum machine learning, I will discuss algorithmic implementations directly aimed at concrete experimental platforms, towards optimal quantum algorithm realizations.

In context of machine-learning assisted interferometry, I will present our work that demonstrates improved interferometer operation aimed towards gravitational wave detection. Here, a key challenge is the reduction of noise of the interferometer mirrors, in particular in-situ. I will discuss our demonstration of in-situ seismic noise reduction, and our way forward.

Invited Talk SYML 1.4 Tue 12:30 E415

Efficient quantum state tomography with convolutional neural networks — •Moritz Reh[1], Tobias Schmale[2], and Martin Gärttner[1,3,4] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany — [2]Institut für Theoretische Physik, Universität Hannover, Welfengarten 1, 30167 Hannover — [3]Physikalisches Institut, Universität Heidelberg, Im Neuenheimer Feld 226, 69120 Heidelberg, Germany — [4]Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg, Germany

Capturing the properties of quantum many-body systems poses a major challenge from a theoretical standpoint, as both the task of numerical simulation as well as the characterization of an experiment from sparse data are suffering from the curse of dimensionality. Variational approaches based on neural networks have therefore become popular, mitigating the curse of dimensionality by searching for a solution in an artificially reduced space. We will motivate and introduce a particular class of such a scheme that allows to describe mixed states in spin systems, before showing its application to quantum state tomography (QST). We show an excellent representability of prototypical ground- and steady states with this ansatz using a number of variational parameters that scales polynomially in system size. This compressed representation allows us to reconstruct states with high classical fidelities outperforming standard methods such as maximum likelihood estimation of the full density matrix.