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Machine-Learning-Enabled Quantum Dynamics and Inverse Materials Design

Reinhard J. Maurer

Department of Chemistry and Department of Physics, University of Warwick, UK

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Location: **Joseph Loschmidt Lecture Hall**
9. Währinger Str. 42, Faculty of Chemistry, ground floor/ intermediate floor

Our ability to discover and design new materials and molecules is being revolutionized by machine-learning (ML) methods. Many approaches use ML to predict materials properties at the level of quantum mechanical (QM) electronic structure theory. This has enabled materials property prediction within vast chemical compound spaces and high-dimensional parametrization of energy landscapes for efficient molecular dynamics simulation of measurable observables. However, as all properties fundamentally derive from the quantum mechanical electronic Hamiltonian of the system, an ML model that can predict said Hamiltonian also has the potential to predict any derived properties while retaining information on the electronic structure.

In this talk, I will introduce data-driven surrogate models of electronic structure with the aim to unlock new materials discovery methods and to achieve greater synergy between physics- and data-driven methods in computational materials science. Using example systems from photocatalysis, organic electronics, and ultrafast dynamics at surfaces, I will discuss the challenges associated with encoding physical symmetries and invariance properties into machine learning models of electronic structure. Once these challenges are overcome, integrated ML-QM methods offer the combined benefits of data-driven parametrization and first-principles-based methods. I will discuss several opportunities associated with building ML-augmented electronic structure methods, including property-driven materials design and the development of efficient and accurate surrogate models that can benefit scientific discovery across a wide range of application areas.

As part of the presentation, there will be a teaching demonstration on the topic "Einstein and Debey Model".