Frontiers of Electronic-Structure Theory: Focus on Artificial Intelligence Applied to Real Materials (SYES)

jointly organised by
the Surface Science Division (O),
the Metal and Material Physics Division (MM),
the Thin Films Division (DS) and
the Semiconductor Physics Division (HL)

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Machine learning methods have gained a prominent spot in the research of materials and molecules, especially in the context of the atomic-scale modeling of their properties. The growing understanding of how machine-learning methods should be adapted to the specific requirements of the field is making them progressively more effective and easy to use. Machine-learning techniques use the predictions of electronic-structure theory to train surrogate models that can compute the same properties with similar accuracy at much reduced cost. The combination of physics-based and data-driven paradigms is extending dramatically the reach of electronic-structure theory, as its predictive accuracy can now be applied to more complex, larger-scale problems and longer timescales. The field has been evolving so fast that in the past years we have witnessed considerable breakthroughs enabled by this combination: first-principles accuracy assessment of finite-temperature thermodynamics, including also subtle effects such as quantum nuclear fluctuations, has become commonplace; predictions of microscopic quantities beyond the interatomic potential energy are making it possible to incorporate functional properties into a fully-predictive machine-learning framework; inverse design and generative models are simplifying the search of configurational and composition spaces for compounds with optimal performance; including information and training data calculated from methods that go beyond density functional theory allows to make predictions systematically improvable.

Overview of Invited Talks and Sessions

(Lecture hall H1)

Invited Talks

SYES 1.1	Thu	15:00–15:30	H1	**Machine-learning-driven advances in modelling inorganic materials** — •Volker L. Deringer
SYES 1.2	Thu	15:30–16:00	H1	**Machine-Learning Discovery of Descriptors for Square-Net Topological Semimetals** — •Eun-Ah Kim
SYES 1.3	Thu	16:00–16:30	H1	**Four Generations of Neural Network Potentials** — •Jörg Behler
SYES 1.4	Thu	16:30–17:00	H1	**Using machine learning to find density functionals** — •Kieron Burke
SYES 1.5	Thu	17:00–17:30	H1	**Coarse graining for classical and quantum systems** — •Cecilia Clementi

Sessions

SYES 1.1–1.5	Thu	15:00–17:30	H1	**Frontiers of Electronic-Structure Theory: Focus on Artificial Intelligence Applied to Real Materials**

Continuation as topical session in O

O 43.1–43.10	Wed	10:30–13:00	S054	**Frontiers of Electronic Structure Theory: Focus on Artificial Intelligence Applied to Real Materials 1**

O 50.1–50.12	Wed	15:00–18:00	S054	**Frontiers of Electronic Structure Theory: Focus on Artificial Intelligence Applied to Real Materials 2**
O 67.1–67.9	Thu	10:30–12:45	S054	**Frontiers of Electronic Structure Theory: Focus on Artificial Intelligence Applied to Real Materials 3**
O 83.1–83.10	Fri	10:30–13:00	S054	**Frontiers of Electronic Structure Theory: Focus on Artificial Intelligence Applied to Real Materials 4**

SYES 1: Frontiers of Electronic-Structure Theory: Focus on Artificial Intelligence Applied to Real Materials

Time: Thursday 15:00–17:30 Location: H1

Invited Talk SYES 1.1 Thu 15:00 H1

Machine-learning-driven advances in modelling inorganic materials — •Volker L. Deringer — University of Oxford, Oxford, UK

Understanding the links between structures and properties of materials is an important research challenge. Computer simulations based on quantum-mechanical methods give access to small-scale models, but quickly reach their limits when structurally complex systems are to be studied. Here, I will showcase recent advances in modelling inorganic functional materials that have been enabled by machine learning (ML) based interatomic potentials. Specifically, I will demonstrate the power of ML-driven simulations in exploring the structures of amorphous elemental systems, at ambient and high pressure, and I will discuss future perspectives for modelling compositionally more complex materials.

Invited Talk SYES 1.2 Thu 15:30 H1

Machine-Learning Discovery of Descriptors for Square-Net Topological Semimetals — •Eun-Ah Kim — Cornell University, Ithaca, NY, USA

The accumulation of massive amounts of materials data motivates data-based machine learning(ML) approaches. However, an extensive database of materials relying on high-throughput density functional theory (DFT) can be unreliable for emergent properties. Much needed is an approach that can articulate and build on expert human researchers' insights. The tolerance factor introduced in Refs [1-2] articulates a chemical insight for identifying topological semimetals among square-net materials and presents an opportunity to develop such a human-machine synergy. Hence, we developed a supervised-unsupervised hybrid approach combining non-linear Gaussian Process(GP) regression [3] with supervised metric learning to discover descriptors for topological semimetals. Simultaneously, we curated a database containing 1279 square-net materials featuring different physical and chemical attributes and the binary label for the topological property associated with each material. Application of the GP model to the database rediscovers the tolerance factor and offers new theoretical insight.

[1] Klemenz, et al, J. Am. Chem. Soc. 2020, 142, 13, 6350-6359

[2] Klemenz, et al, Annual Review of Materials Research 2019 49:1, 185-206

[3] D. Milios, et al, Advance in Neural Information Processing Systems, page 11,2018

Invited Talk SYES 1.3 Thu 16:00 H1

Four Generations of Neural Network Potentials — •Jörg Behler — Universität Göttingen, Germany

A lot of progress has been made in recent years in the development of machine learning potentials for atomistic simulations, with neural network potentials (NNPs) being an important example. While the first generation of NNPs has been restricted to small systems, the second generation extended the applicability of ML potentials to high-dimensional systems containing thousands of atoms by constructing the total energy as a sum of environment-dependent atomic energies. Long-range electrostatic interactions can be included in third-generation NNPs employing environment-dependent charges, but only recently limitations of this locality approximation could be overcome by the introduction of fourth-generation NNPs, which are able to describe non-local charge transfer using a global charge equilibration step. In this talk an overview about the historical evolution of high-dimensional neural network potentials will be given along with an overview of typical applications in large-scale atomistic simulations.

Invited Talk SYES 1.4 Thu 16:30 H1

Using machine learning to find density functionals — •Kieron Burke — University of California, Irvine, USA

Over the past decade, advances in machine learning have led to the creation of new approximate density functionals. I will review this area, with an emphasis on very recent developments. How do such functionals compare to those of human design? What are their advantages and their limitations? For example, can they work for strongly correlated systems? I will consider both the exchange-correlation energy used in Kohn-Sham DFT and the non-interacting kinetic energy functional, needed to bypass the KS equations.

• How Well Does Kohn-Sham Regularizer Work for Weakly Correlated Systems? B. Kalita, R. Pederson, J. Chen, L. Li, and K. Burke, J. Phys. Chem. Lett (2022).

• Machine learning and density functional theory R. Pederson, B. Kalita, and K. Burke, Nat. Rev. Phys. (2022).

• Kohn-Sham Equations as Regularizer: Building Prior Knowledge into Machine-Learned Physics L. Li, S. Hoyer, R. Pederson, R. Sun, E. Cubuk, P. Riley, and K. Burke, Phys. Rev. Lett. 126, 036401 (2021).

• Using Machine Learning to Find New Density Functionals B. Kalita and K. Burke, Article in Roadmap on Machine Learning in Electronic Structure (2022).

Invited Talk SYES 1.5 Thu 17:00 H1

Coarse graining for classical and quantum systems — •Cecilia Clementi — Freie Universität Berlin, Germany

The last years have seen an immense increase in high-throughput and high-resolution technologies for experimental observation as well as high-performance techniques to simulate molecular systems at a microscopic level, resulting in vast and ever-increasing amounts of high-dimensional data. However, experiments provide only a partial view of the molecular processes and are limited in their temporal and spatial resolution. On the other hand, simulations are still not able to completely characterize large and/or complex molecular processes over long timescales, thus leaving significant gaps in our ability to study these processes at a physically relevant scale. We present our efforts to bridge these gaps, by combining statistical physics with state-of-the-art machine-learning methods to design optimal coarse models for complex macromolecular systems. We derive simplified molecular models to reproduce the essential information contained both in microscopic simulation and experimental measurements.