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**