NUS National University of Singapore | Department of Materials Science & Engineering
College of Design and Engineering

Department Seminar

Dear Colleagues & Students,
You are cordially invited to a special seminar on

Errors that matter: Uncertainty-aware universal machine-learning potentials calibrated on experiments

Date: 19th Jun 2026 (Fri) ; Time: 9 am – 11 am

Venue: Block EA, level 6, EA-06-03 (NUS Campus Map)

By Prof Michele Ceriotti

Institute of Materials, EPFL, Switzerland

Hosted by Prof Ong Shyue Ping

Abstract:

Machine-learning models of atomic-scale interactions achieve the accuracy of the quantum mechanical calculations on which they are trained, but at a dramatically lower computational cost. While traditionally they have been trained for specific systems and thermodynamic conditions, recent work have shown extraordinary levels of transferability, with e.g. the PET-MAD-1.5 model delivering stable molecular dynamics for diverse types of configurations involving any of the first 102 elements of the periodic table, from H to No. This broad transferability calls for reliable uncertainty quantification. Thanks to graph-sharing ensembles and thermodynamic reweighting, it is possible to estimate the error of a simulation using a MLIP against that using the quantum mechanical method it is trained on. These errors, however, do not include uncertainty contributions from the approximations inherent in the electronic structure reference, which are often the main source of discrepancy with empirical observations.
Here I present PET-EXP, a model that combines shallow ensembles and statistical reweighting with uncertainty-aware functional distributions, and using models trained on different flavors of density functional theory calibrated against experiments. I will show that this approach allows predicting end-to-end modelling errors relative to experimental measurements at virtually no additional cost over a simulation based on a single conventional ML potential - not only for the properties used for calibration, but also more complicated simulation outputs such as mean densities and radial distribution functions of liquids. Ultimately, this framework provides a practical and inexpensive approach to elevate machine-learning potentials from faithful interpolators of approximate theories to genuinely predictive tools anchored in experimental reality.

Biography:

Michele Ceriotti is a professor at EPFL, where he leads the laboratory for Computational Science and Modelling and directs the Institute of Materials. His research interests are rooted in the atomistic-scale modelling of matter bridging quantum mechanics, statistical physics and machine learning. He has contributed modelling insights into several classes of materials, from water and aqueous systems to molecular crystals, functional materials, metallic alloys and high-entropy compounds. He is a vocal advocate of open science and open software, leading the development of several open-source modelling tools including http://metatensor.org, http://ipi-code.org and http://chemiscope.org.

Looking forward to seeing all of you!