TAU Center for AI and Data Science (TAD) Physical Sciences Community in Collaboration with the School of Chemistry, Sackler Center for Computational Molecular and Material Sciences & Ratner Center for Single Molecule Science are inviting you to a special tutorial and seminar by

Prof. Michele Ceriotti

Laboratory of Computational Science and Modelling, EPFL

- ## Workshop: Equivariant machine learning - a tutorial introduction

June 7, 11:00 – 13:00, The Multidisciplinary Building #315

As with many fields of science, machine learning methods have become an essential part of the toolbox for modeling matter at the atomic scale, with many frameworks having become well-established, and many more being developed in new research directions. Lately, much effort has been dedicated to rationalizing the relationship between models of atomic-scale properties and fundamental physical principles, such as symmetry, locality, and hierarchical decompositions of the interactions between atoms.

I will present an overview of the latest developments, focusing in particular on the problem of *representing* an atomic structure and its properties in a concise, yet complete, fashion. I will provide an introduction to the concept of equivariance (i.e. building models that are consistent with a prescribed set of symmetries), explaining how it underpins most of the last-generation models, and showing practical examples of equivariant models in action.

Advanced registration is required. **Please REGISTER HERE.**

- ## Seminar: Atomic-scale modeling in the age of machine learning

June 9, 15:00, The Multidisciplinary building #315

When modeling materials and molecules at the atomic scale, achieving a realistic level of complexity and making quantitative predictions are usually conflicting goals. Data-driven techniques have made great strides towards enabling simulations of materials in realistic conditions with uncompromising accuracy.
In this talk I will summarize the core concepts that have driven the extraordinarily fast progress of the field, discuss some of the most promising modeling techniques that combine physics-inspired and data-driven paradigms, indicate the most pressing open challenges, and present several compelling examples ranging from water to semiconductors and from metals to molecular materials.

See Michele Ceriotti's Biography here: https://people.epfl.ch/michele.ceriotti?lang=en