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SEMINAR SERIES

HIGHLIGHTS IN ENERGY RESEARCH

08.11.2018, 16:00 - 17:00, EPFL Valais, 4th floor, ZEUZIER room

Machine Learning Like a Physicist

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Host : Prof. Wendy Queen

Statistical regression techniques have become very fashionable as a tool to predict the properties of systems at the atomic scale, sidestepping much of the computational cost of first-principles simulations and making it possible to perform simulations that require thorough statistical sampling without compromising on the accuracy of the electronic structure model.
In this talk I will argue how data-driven modelling can be rooted in a mathematically rigorous and physically-motivated framework, and how this is beneficial to the accuracy and the transferability of the model. I will also highlight how machine learning - despite amounting essentially at data interpolation - can provide important physical insights on the behavior of complex systems, on the synthesizability and on the structure-property relations of materials.
I will give examples concerning all sorts of atomistic systems, from semiconductors to molecular crystals [1], and properties as diverse as drug-protein interactions [2], dielectric response of aqueous systems[3] and NMR chemical shielding in the solid state [4].

[1] F. Musil, S. De, J. Yang, J. E. J. E. Campbell, G. M. G. M. Day, and M. Ceriotti, Chem. Sci. 9 (2018) 1289
[2] A. P. A. P. Bartók, S. De, C. Poelking, N. Bernstein, J. R. J. R. Kermode, G. Csányi, and M. Ceriotti, Sci. Adv. 3, (2017) e1701816
[3] A. Grisafi, D. M. Wilkins, G. Csányi, and M. Ceriotti, Phys. Rev. Lett. 120 (2018) 36002
[4] http://shiftml.

Bio:
Michele Ceriotti received his Ph.D. in Physics from ETH Zürich. He spent three years in Oxford as a Junior Research Fellow at Merton College, funded from a Royal Society Newton Fellowship and a Marie Curie Fellowship. Since 2013 he works as an assistant professor at the Institute of Materials at EPFL, leading the laboratory for Computational Science and Modeling. His research interests focus on the development of methods for molecular dynamics and quantum simulations of hydrogen-bonded materials, machine-learning study of complex systems at the atomistic level, and on their application to problems in chemistry and materials science. He has been awarded the IBM Research Forschungspreis in 2010, the Volker Heine Young Investigator Award in 2013, an ERC Starting Grant in 2016, and the IUPAP C10 Young Scientist Prize in 2018.