

CIS - "Get to know your neighbors" Seminar series # 3

Abstract

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Physics-inspired Machine Learning for Materials Discovery

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Machine learning is making its way into all fields of science, and it is clear that - beyond the hype - it provides useful approaches that will change the way both experiment and modelling are performed. In particular, 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 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 can provide important physical insights on the behavior of complex systems, and on the structure-property relations of materials.