MARVEL

NATIONAL CENTRE OF COMPETENCE IN RESEARCH

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

NCCR MARVEL Distinguished Lecture

Machine-learning of density functionals for applications in molecules and materials

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Tuesday 20 February 2018, 16:15, Room MXF1

Abstract: This lecture is designed to be accessible to a wide variety of backgrounds.

In the first part, I will briefly review density functional theory and why it is important to many branches of modern physical science. I will also review machine learning and its recent applications to molecules and materials.

In the second half, I will show how, in collaboration with computer scientists at TU Berlin, we have used a specific type of machine-learning, called kernel ridge regression, to find more accurate and powerful approximate density functionals than any made by humans.

For more background, see here.

FNSNF Swiss National Science Foundation

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