Lecture within the International Graduate Summer School – Modeling and Simulations Across the Molecular Sciences and Engineering

Joint with the Centre for Research in Molecular Modeling (CERMM) Seminar Series

July 12, 2019, 2 :30 PM – GE-110

Sergei Manzhos

Institut National de la Recherche Scientifique

Machine Learning in the Context of Atomistic Simulations

I will present the case for and examples of the use of machine learning (ML) techniques for atomistic simulations, including solutions of the electronic problem as well as nuclei dynamics. I will introduce approaches such as neural networks, dimensionality reduction, Gaussian process regressions, generic algorithms and discuss pros and cons and comparisons of them in the context of recovering input-output relations in multidimensional spaces from sparse data. I will show how ML is used to build potential energy surfaces for molecules and interfaces from sparse data and in quantum-dynamic friendly form, to construct kinetic energy functionals and local pseudopotentials for orbital-free DFT, and to help solve the Schroedinger equation, including direct representation of wavefunctions and representation of the potential function in a non-quadrature based approach.

Sergei Manzhos is Associate Professor at the Centre Énergy Matériaux Télécommunications (EMT) of the Institut National de la Recherche Scientifique (INRS). He holds Ph.D. in chemistry from Queen's University (2005) and M.Sc. In radio physics from Kharkiv National University (1999). In 2004-2008 he was postdoctoral fellow and NSERC postdoctoral fellow at the Université de Montréal in the group of Prof. Tucker Carrington. He was Project Assistant Professor at the University of Tokyo (Department of Chemical System Engineering and Research Centre for Advanced Science and Technology) in 2008-2012, working in groups of Prof. Koichi Yamashina and Prof. Hiroshi Segawa. In 2012-2019, he was Assistant Professor (group leader) at the Department of Mechanical Engineering, National University of Singapore before joining INRS in 2019.

Prof. Manzhos's research interests include computational materials modeling and design for energy conversion and storage technologies as well as method development for computational spectroscopy and large-scale ab initio methods. He uses and develops machine learning based methods for this applications.