

# nanoSeminar Series 2022

Institute for Materials Science

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Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg

**Physics-inspired machine learning force fields for flexible molecules**

Thursday, September 22<sup>nd</sup> 2022  
13:00 – 14:00

Normal: Seminar Room 115, Hallwachsstr. 3 (HAL)  
Pandemic version: <https://tinyurl.com/nanoSeminar-GA>

In recent years, the use of machine learning (ML) in computational chemistry has enabled numerous advances previously out of reach due to the computational complexity of traditional electronic-structure methods. One of the most promising applications is the construction of ML-based force fields (FFs), with the aim to narrow the gap between the accuracy of ab initio methods and the efficiency of classical FFs. This has provided a tool for computing several physicochemical properties that would require millions of CPU years otherwise. The key idea is to learn the statistical relation between chemical structure and potential energy without relying on a preconceived notion of fixed chemical bonds or knowledge about the relevant interactions. However, many successful applications of MLFFs have been restricted to small-and medium-sized molecules. This seminar gives an overview of the core concepts underlying ML-FFs and discusses the challenges for the generation of MLFFs of more flexible and complex molecular systems.

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Leonardo Medrano is currently working as a postdoctoral researcher at the group of Prof. Alexandre Tkatchenko at the University of Luxembourg. He is combining machine learning methods with quantum/statistical mechanics to develop transferable/scalable physics-inspired neural network potentials for the study of drug-protein interactions as well as frameworks for computer-aided molecular design. In 2018, Leonardo got his doctor degree in Mechanical Engineering under the supervision of Prof. Gianauelio Cuniberti at the Technical University of Dresden as an IMPRS fellow (International Max Planck Research School). There, he carried out several atomistic investigations to gain insights on the electron and thermal transport properties of novel low-dimensional materials. Earlier, he got his bachelor and master's degree in Physics at the National University of San Marcos in Lima-Peru. Besides his theoretical investigations, Leonardo is also interested in multi-disciplinary projects involving experimental/industrial collaborators to deal with current challenges in Physics and Chemistry (see google scholar page).