Workshop: Parametrization with the Amsterdam Modeling Suite

Presented by Software for Chemistry & Materials

In this workshop, we will introduce the Amsterdam Modeling Suite to perform atomistic simulations of molecules, solids and interfaces, focusing on the development of accurate interatomic potentials. First, you will learn how to use the graphical user interface to setup, manage and analyze calculations based on density functional theory, classical and semi-empirical methods. Second, you will learn how to use our parametrization tool ParAMS to optimize parameters for DFTB and ReaxFF. For example, you will learn how to prepare the data set, select the proper parameters to optimize, and understand the optimization algorithms. Third, you will discover our new extension for ParAMS to optimize Machine Learning Potentials (MLP). This new tool allows you to train M3GNet from scratch, or using transfer learning to fine-tune the universal parameters, as well as to train committees, to access uncertainties of the model. Finally, you will learn how to perform active learning to create an MLP that will automatically learn from a targeted molecular dynamics simulation.

This 1-day, in-person workshop will be composed of lecture sessions where our experts from Software for Chemistry & Materials will present the theory behind the various levels of theory approached, together with hands-on tutorials where you will prepare and train ReaxFF, DFTB and MLP models with ParAMS.

Our team from SCM will be composed of:

Dr. Nicolas Onofrio – Technical Sales Representative. Before joining SCM in 2023, Nicolas obtained his PhD at the Université Grenoble Alpes, he was a visiting Assistant Professor at Purdue University, and an Assistant Professor at the Hong Kong Polytechnic University. He has been working on various topics related to modeling electrochemical interfaces with applications to electronics and catalysis. At SCM, Nicolas is using his wide experience in atomistic simulations to help researchers make their best use of the Amsterdam Modeling Suite.

Dr. Paul Spiering – Software Developer. Paul has obtained his PhD with successfully modeling non-adiabatic effects for molecule-surface reactions in the theoretical chemistry group of Geert-Jan Kroes under the supervision of Jörg Meyer. In particular, a machine learning method for equivariant tensors was developed. Paul joined SCM in 2022 to work on enhancing the machine learning capabilities of the Amsterdam Modeling Suite.

References:

Software for Chemistry & Materials https://www.scm.com
ParAMS https://www.scm.com/product/params
MLP https://www.scm.com/doc/MLPotential

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