Modelling of Complex Energy Materials with Machine Learning

Nongnuch Artrith*

Materials Chemistry and Catalysis, Debye Institute for Nanomaterials Science,
Utrecht University, The Netherlands
*E-mail: n.artrith@uu.nl

The properties of materials for energy applications, such as heterogeneous catalysts and battery materials, often depend on complicated chemical compositions and complex structural features including defects and disorder. This complexity makes the direct modelling with first principles methods challenging. Machine-learning (ML) potentials trained on first principles reference data enable linear-scaling atomistic simulations with an accuracy that is close to the reference method at a fraction of the computational cost. ML models can also be trained to predict the outcome of simulations or experiments, bypassing explicit atomistic modelling altogether.

Here, I will give an overview of our contributions to the development of ML potentials based on artificial neural networks (ANNs) [1-3] and applications of the method to challenging materials classes including metal and oxide nanoparticles, amorphous phases, and interfaces [4-5]. Further, I will show how large computational and small experimental data sets can be integrated for the ML-guided discovery of catalyst materials [6]. These examples show that the combination of first-principles calculations and ML models is a useful tool for the modelling of nanomaterials and for materials discovery. All data and models are made publicly available. To promote Open Science, we also formulated guidelines for the publication of ML models for chemistry that aim at transparency and reproducibility [7].

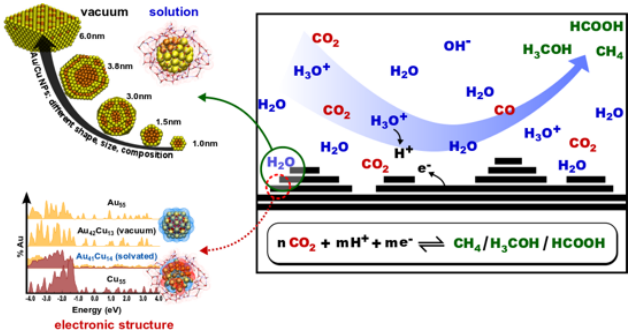

Figure 1. Electrochemical Interfaces: Complex Systems are Challenging for Simulations.

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