UNIVERSITÄT DUISBURG ESSEN

PHYSIK E=

Physikalisches Kolloquium

Mittwoch, 28.05.2025
13:00 Uhr
MC 122 und Zoom

https://uni-due.zoom-x.de/j/64228670246?pwd=RjVQeFNIUkRKRkpiNVpKYXhJaFNLdz09 (gilt für alle Vorträge)

Atomistic Simulations of Complex Systems with High-Dimensional Neural Network Potentials

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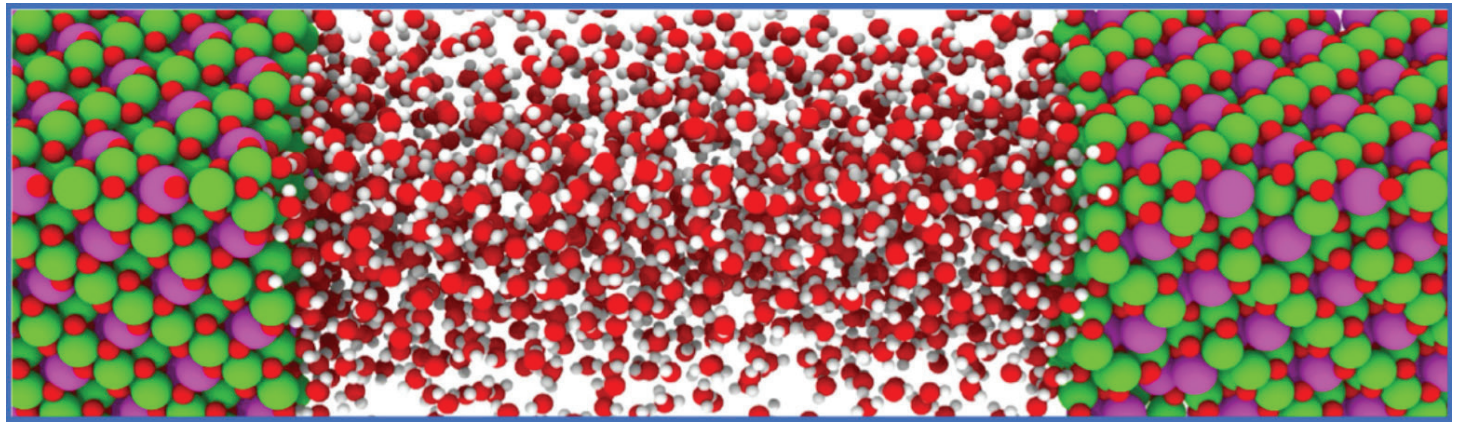

In recent years there has been tremendous progress in the development of interatomic potentials employing machine learning. High-dimensional neural network potentials (HDNNP) are an important class of machine learning potentials, which allow to combine the accuracy of electronic structure calculations with the efficiency of simple empirical potentials enabling large-scale simulations. Depending on the types of systems and physical phenomena they are able to describe, HDNNPs can be classified into up to now four generations. In this talk, an overview about the methodical evolution of HDNNPs will be given along with typical example applications to condensed systems with a particular focus on chemical processes at solid-liquid interfaces.