This lecture will introduce a few different types of machine learning potentials for describing potential energy surfaces. In particular, high-dimensional neural network potentials can be quickly evaluated and are thus suitable for large-scale molecular dynamics simulations. Several aspects will be covered, including the selection of training data, the training procedure, validation, examples from the literature, and remaining methodological challenges.

In the hands-on session, the participants parameterize their own simple neural network potential for a simple system using open-source Python packages. A basic knowledge of Python is required to be able to appreciate the hands-on session.