

## COMPUTING@PNNL SEMINAR SERIES PRESENTS

Prof. Dr. Jörg Behler



# Understanding Complex Systems with High-Dimensional Neural Network Potentials

A lot of progress has been made in recent years in the development of atomistic potentials employing machine learning (ML). Neural network potentials (NNPs), which were first proposed about two decades ago, are an important class of ML potentials. While the first NNPs were restricted to small molecules with only a few degrees of freedom, they are now applicable to high-dimensional systems containing thousands of atoms, which enables addressing a variety of problems in chemistry, physics, and materials science. In this talk, the main concepts of NNPs will be presented, with a special focus on constructing NNPs for high-dimensional condensed systems.

Jörg Behler graduated in chemistry at the University of Dortmund in 2000. In 2004, he obtained his PhD at the Fritz-Haber-Institute in Berlin. For his thesis on the interaction of oxygen molecules with aluminum surfaces, he was awarded the Otto-Hahn medal of the Max-Planck society. After a postdoctoral stay at the ETH Zürich, in 2007 he established his own research group at the Ruhr-Universität Bochum funded by a Liebig, an Emmy Noether, and a Heisenberg fellowship of the German Science Foundation. In 2013, he received the Hans G. A. Hellmann award for his work on the development of high-dimensional neural network potentials. He obtained his *venia legendi* in theoretical chemistry in 2014 and has been a full professor for theoretical chemistry at the University of Göttingen since 2017.

**Tuesday, August 11**  
**11:00am – 12:00pm**  
**Zoom Webinar**

<https://pnnl.zoomgov.com/j/1600108006?pwd=NkMrM0wxRE4zbTZBSVVwN3BFdzFodz09>