

Impact, Uncertain Expectations, and Open Challenges of AI in Materials Science

Matthias Scheffler

The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, Berlin, Germany

The function of materials is typically ruled by a high intricacy of various processes, making explicit *ab initio* modeling often too complicated or even unrealistic.

Machine learning and AI enable the prediction of mean values and probability distributions of a material's function by addressing correlations, smoothing out the detailed microscopic physics and chemistry. In this talk, I will discuss some recent examples, also addressing the frequently-ignored uncertainty of AI predictions. Often, material functions are triggered by rare events that may be absent in the training data, smoothed away by regularization, or fake events may be predicted. I will discuss how this challenge can be solved, and I will explore how machine learning can identify "rules" and "materials genes", enabling active learning for systematic, efficient predictions of novel materials with improved functional performance.