UNIVERSITÄT DUISBURG ESSEN

PHYSIK E=

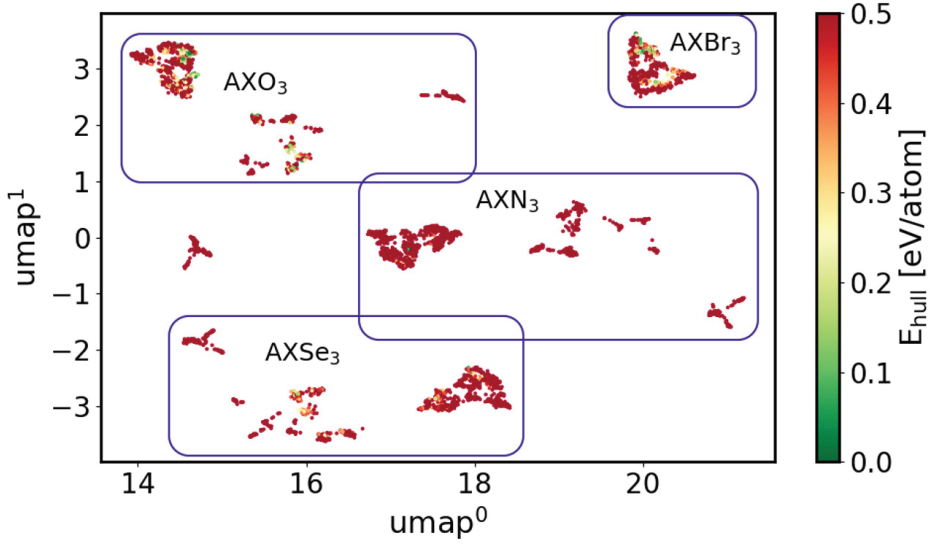
Physikalisches Kolloquium

Mittwoch, 02.07.2025
13:00 Uhr
MC 122 und Zoom

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

Machine Learning for Materials Design: From Materials Databases to Predictive Insights

Prof. Dr. Silvana Botti, Faculty of Physics and Astronomy, Ruhr Universität Bochum



Machine learning approaches have revolutionized materials discovery by enabling efficient exploration of vast chemical spaces for targeted applications. In this presentation, we demonstrate how the synergy between high-throughput computational screening and machine learning accelerates the design of novel functional materials. By integrating machine learning algorithms with density-functional theory calculations, we have developed frameworks that significantly reduce computational costs while maintaining predictive accuracy. We present our recent breakthroughs in discovering and characterizing promising inorganic compounds for energy applications.

Beyond bulk properties, we address the critical role of interfaces in electronic devices such as transistors or solar cells. These interfaces enable the exploitation of quantum processes through engineered potential gradients that can manipulate electron behavior in multilayer systems. We showcase our approaches to interface design and characterization, overcoming limitations in current methodologies and opening new possibilities for the computational design next-generation energy materials and devices.