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Machine-Learning-Assisted Design of Materials for Energy

In this presentation, we explore the utilization of supercomputers to design new functional materials with a focus on energy applications. The combination of high throughput techniques and rapidly advancing supercomputers enables the automatic screening of vast numbers of hypothetical materials, providing solutions to current technological challenges. Moreover, the integration of machine learning methods with density-functional theory offers a powerful approach to accelerate materials discovery. We summarize our recent efforts in the discovery, characterization, and understanding of inorganic compounds using these innovative approaches, with a specific emphasis on materials for photovoltaics.

While characterizing the electronic properties of crystalline bulk materials is crucial, it may not be sufficient when considering electronic devices. Interfaces, such as those found in transistors, light-emitting diodes, and solar cells, play a pivotal role in exploiting quantum processes involving electrons in tailored multilayers. The ability to shape potential gradients at interfaces opens up opportunities for electron manipulation and the development of new functionalities. However, designing interfaces and gaining a deep understanding of their properties present challenges that exceed the current state of the art. We discuss recent advancements in this direction.