

High Performance Computing and Materials Science: How atomistic simulations can pave the way for clean and sustainable energy

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The availability of cheap and abundant energy was one of the main drivers of the industrial revolution. Until today, energy remains an essential ingredient for many aspects of human activity. It is recognized that a major challenge of our times is the transition towards sustainable energy conversion, moving away from carbon-based fossil fuels. Developing more efficient and cheaper ways to convert wind or solar radiation into electricity or to store electric energy are important steps in this transition.

Computer simulations at the atomic scale can lead to a detailed understanding of the fundamental steps during energy conversion. In this presentation, I will illustrate a few cases where such a “computational microscope” can be used by materials scientists to develop better solar cells or to more efficiently use solar light to split water into hydrogen and oxygen. In these cases, high performance computing allows for a screening of potential materials, before they have even been synthesized in a laboratory.

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