

Special Issue

Molecular Scale Research of Energy Materials

Message from the Guest Editor

The envisaged green transition will require, for being sustainable, the design of new materials. It involves the collection, storage, and conversion of energy, which has led to the research of a series of energy materials, such as photocatalytic materials, perovskite materials, lithium battery materials, biomass energy materials, etc.

Although the actual functioning of energy devices occurs at the macroscopic scale, this is due to chemical and physical processes originating at the molecular scale. The periodic crystalline unit comprising up to a few tens of atoms determines light absorption and charge transport. Free energy surfaces of a molecular complex in proximity to a surface determine its catalytic activity. This Special Issue is focused on experimental and theoretical/computational contributions tackling the properties at the molecular scale of the extended family of energy materials. It focuses on the latest research on energy materials from the molecular scale to the design and synthesis of energy materials, electron and ion transport mechanisms, catalytic activity, and energy conversion mechanisms.

Guest Editor

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