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Special Issue on

Computational Approaches to Energy Storage Materials: Theory, Methodology, and Applications

CALL FOR PAPERS

The importance of efficient and clean energy has grown enormously over the past decades, driven by the threats of global warming, environmental pollution, and the need for energy security. Energy that is based on electricity generated from renewable sources offers enormous potential for meeting future energy demands. However, these renewable sources require efficient electrical energy storage due to their intrinsic limits: variability and uncertainty. Also, state-of-the-art electric vehicles are not competitive with gasoline powered vehicles. New materials and systems that can show higher energy and power densities than those found in current systems are required for plug-in hybrid-electric vehicles (PHEVs) and all-electric vehicles (EVs) to be broadly competitive.

Although energy storage devices have shown significant progress over many decades, there are still fundamental gaps in the understanding of physical processes that govern their operation, performance, and failure. Fundamental research is critically needed to uncover the underlying principles that govern these complicated and interrelated processes. With a full understanding of these processes, new ideas can be formulated to address energy storage technology gaps and to meet future energy storage demands.

We solicit high quality, original research articles as well as review articles that focus on the computational modeling and simulation applied in the field of energy materials. They should have a sustainable and important impact on the development of new directions in theory and methodology as well as potential applications.

Potential topics include, but are not limited to:

- First principles/atomistic computational approaches to determine the structure or properties of energy storage materials
- Mesoscale simulations to investigate the transport and reaction properties of energy storage systems
- Multiscale models linking different scales
- Degradation models that focused on mechanical/chemical/thermal aspects and their coupling effects
- Simplified electrochemical models for control-oriented purposes

Authors can submit their manuscripts via the Manuscript Tracking System at http://mts.hindawi.com/submit/journals/jchem/physical.chemistry/caesm/.

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