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TMS 2017
146th Annual Meeting & Exhibition



February 26 – March 2, 2017
San Diego, California, USA

COMPUTATIONAL APPROACHES TO MATERIALS FOR ENERGY APPLICATIONS

During the last few years, theoretical approaches to materials for energy applications, like solar energy conversion and thermoelectricity, have become more quantitative. For example, they allow researchers to guide experiments through a very detailed understanding of the underlying mechanisms, or even through the screening of a large number of compounds to find new materials with specific properties.

The purpose of this symposium is to highlight the recent computational advances which would find application in the search for new materials and devices for energy applications. Therefore, the topics for this year will include:

- Transport theory
- Many body perturbations theory for electrons and phonons
- Multiscale modeling
- Datamining

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