4th International Symposium on
Energy Challenges & Mechanics
- working on small scales

11-13 August 2015
Aberdeen, Scotland, UK

Heterogeneous Nano-Material Design for Energy Conversion and Storage

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Accepted for publication on 27th June 2015

Heterogeneous functional materials with functional void phases and surfaces, e.g., HeteroFoaM materials, are critical elements of many energy conversion and storage devices including batteries, fuel cells and flow batteries, separation membranes, and capacitive devices. Such materials are typically multifunctional, and their reaction with applied mechanical, electrical, and thermal fields is the subject of design for performance. That design enterprise involves the constituents, their morphologies, and their interfaces and surfaces. The purpose of this session is to define the challenges and to identify the best approaches to achieving an understanding, constructing models and analysis, and predicting behavior of such heterogeneous systems as a genre of materials. Fundamentals will be emphasized, but applications and demonstrations of the concepts will be featured as well.

The "cost" of energy is determined by the collective expense of converting it to useful forms, something we call "using energy," even though we cannot destroy or create it. Recently there has been much discussion of an "energy cliff," based on the reality that converting and storing new sources of energy (such as shale gas, etc.) may incur costs that are greater than the benefit we subsequently derive from them. This, in turn, has driven the need for improving efficiency in our energy systems and the need for energy conversion and storage devices that are capable of operating on a diverse supply of fuel, including legacy supplies.

The present discussion with focus on the design of the heterogeneous membranes, electrodes, and systems that make that possible. Technical issues discussed will include methods of resolving and rendering internal detail in heterogeneous energy materials, multi-scale, multiphysics conformal modelling and design of morphology driven by species flux balance, uncertainty and validation of simulation models, and demonstration of first-principles concepts for heterogeneous materials for conversion and storage.

Keywords: heterogeneous; energy materials; conversion; storage