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Succeeding with New Energy Materials: A Market-Driven Modeling Approach

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Abstract:

There is an increasing need within energy, resource, and manufacturing industries to assess the relative competitive potential of new chemical processes, materials, and technology. Despite such potentials, the deployment of cost-competitive, highly efficient materials for renewable energy conversion and storage technologies faces enormous challenges [1,2]. For large-scale commercialization of electrochemical energy devices, manufacturers need to develop low cost materials and fabrication approaches that preserve current levels of performance and stability [3].

In this presentation, we focus on electrochemical materials fabrication process for polymer electrolyte fuel cells and electrochemical batteries. We discuss case studies of how integrating computer simulations with cost modeling methodologies in the context of a new innovation can greatly assist in optimizing efforts and investment on developing new electrochemical materials [4].

At the materials modeling side, mesoscale simulations are employed to allow evaluating key factors during fabrication process by unravelling the overall relations between chemistry, structure, and performance. Such models provide relations between structure, properties, and performance that could potentially optimize device operation. These computational models should be fine-tuned to inform the materials design in view of ease of fabrication, cost, integration and performance of new generation of components. Building upon meso-scale modeling and lab-scale fabrication processes, the cost modeling quantifies the materials fabrication costs and potential techno-economic benefits associated with the medium to large-scale manufacturing of the new materials. We finally propose an R&D investment methodology for new electrochemical materials development to reduce risk and shorten time to market.

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