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Computational materials design for energy applications¹

VIDVUDS OZOLINS, Department of Materials Science and Engineering, University of California, Los Angeles, California 90095-1595, USA

General adoption of sustainable energy technologies depends on the discovery and development of new high-performance materials. For instance, waste heat recovery and electricity generation via the solar thermal route require bulk thermoelectrics with a high figure of merit (ZT) and thermal stability at high-temperatures. Energy recovery applications (e.g., regenerative braking) call for the development of rapidly chargeable systems for electrical energy storage, such as electrochemical supercapacitors. Similarly, use of hydrogen as vehicular fuel depends on the ability to store hydrogen at high volumetric and gravimetric densities, as well as on the ability to extract it at ambient temperatures at sufficiently rapid rates. We will discuss how first-principles computational methods based on quantum mechanics and statistical physics can drive the understanding, improvement and prediction of new energy materials. We will cover prediction and experimental verification of new earth-abundant thermoelectrics, transition metal oxides for electrochemical supercapacitors, and kinetics of mass transport in complex metal hydrides.

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