

Computational Approaches for Investigating Electrochemical Energy Storage Materials and Devices

Sreekanth Pannela, Bobby G. Sumpter, and Paul Kent Oak Ridge National Laboratory

Large-scale computational simulations at the quantum and atomistic level are used to explore interfacial processes between electrolytes/electrodes from which models are derived that can help provide guidance towards the design of improved performance. Additionally, by using coarse-grained methods, simulations that couple charge/thermal transport with mechanical and detailed chemical reactions are feasible and can be used to help understand issues such as the thermal runaway under abuse.