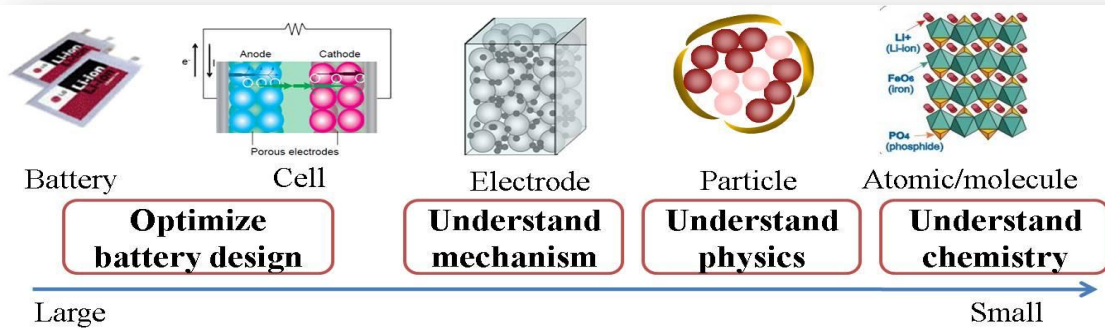
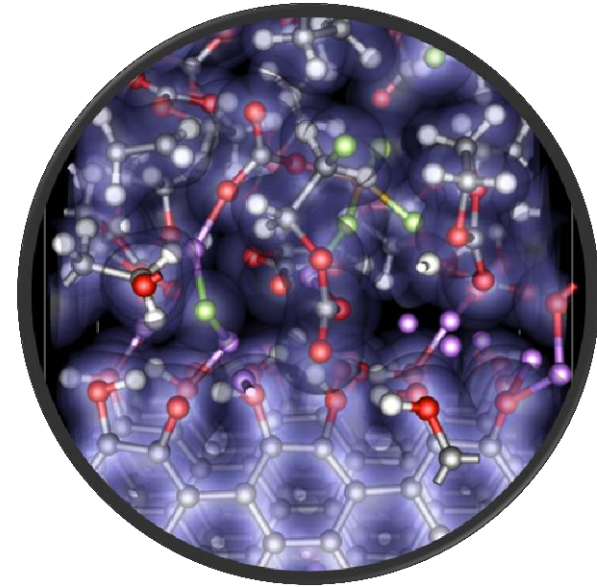


Theory, Modeling, and Simulation: Overview

- Simulations can help accelerate the process of materials discovery by providing atomic level understanding of phenomena and predictions of chemical trends, especially when used in concert with experiments.
- Theory/methods encompassing electrons, atoms, molecules, meso, micro and macroscales
 - Can provide understanding, prediction, and ability for exploration of new materials and conditions before they are realized in the lab
 - Can illuminate connections between experimental observations
 - Can help identify new synthetic pathways



Sumpter, Pannala, Kent and Turner