

First principles modeling of materials for energy storage and conversion applications

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Commercial applications of energy storage and conversion require high-efficiency active functional materials that operate at the core of these systems. First principles atomistic modeling offers ways to gain understanding of fundamental mechanisms that govern how these materials work. This understanding in turn leads to ideas of how to systematically design and improve them, thus making certain technologies feasible and cost-effective. I will give a wide overview of our efforts at Bosch Research in development and applications of efficient first-principles computational methodology development to better understanding of new materials in the following key areas :

- Modeling of electronic and thermal transport in thermoelectric materials
- Discovery and optimization of new materials for Li-ion batteries
- Materials for new concepts beyond Li-ion batteries

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