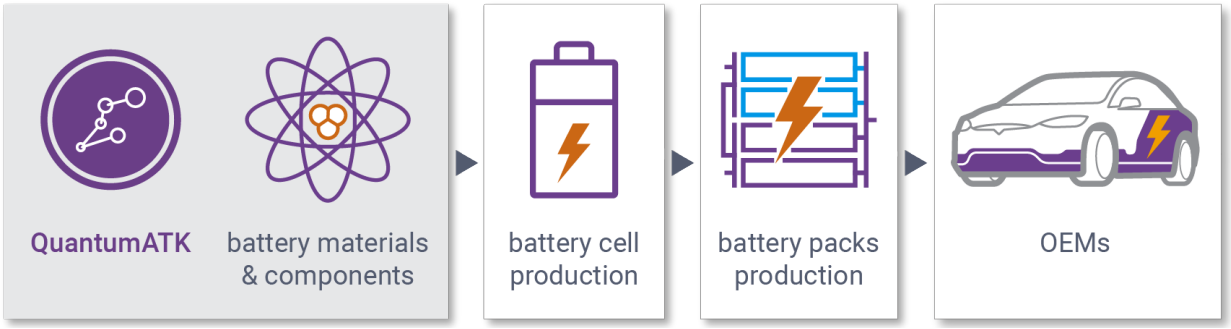
SYNOPSYS®

Battery Material Simulations with QuantumATK

QuantumATK atomistic simulation software is used to design novel battery materials for cathodes and anodes, liquid and solid electrolytes, additives, solid electrolyte interphases (SEI) for denser and safer batteries for automotive and other industrial applications. It enables systematic selection of materials and performance optimization through co-design of structure and chemistry, shortening battery development time and reducing costs.



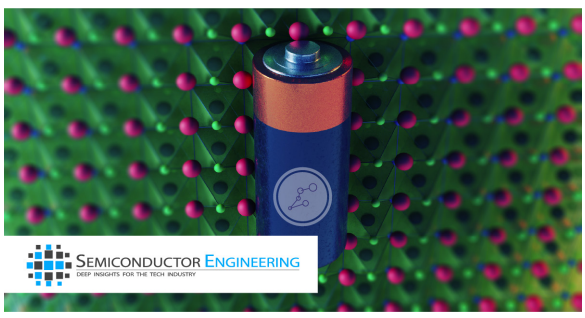
Battery Material Design Directions

Cathode
- Higher capacity and longer cycle life
- Electrochemical stability (surface, bulk)
- Lower scarce and expensive element, e.g., Co, content
- Higher ion diffusivity

Anode
- Suppressed dendrite formation
- Mechanical properties (suppressed swelling, crack formation)
- Electrochemical stability (SEI)
- Graphite, Silicon and Li-metal anodes

Electrolyte
- Higher ion diffusivity at a wide range of temperatures
- Electrochemical stability
- Non-flammable

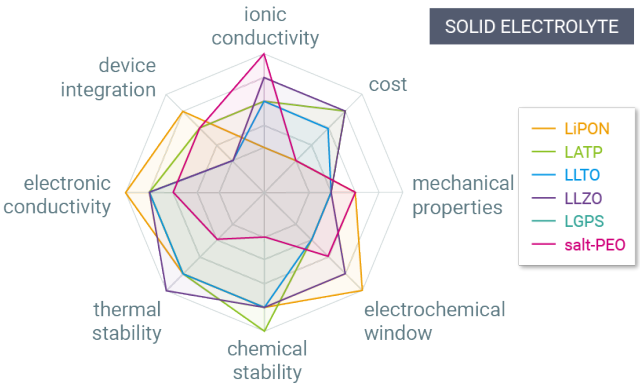
Interfaces between materials

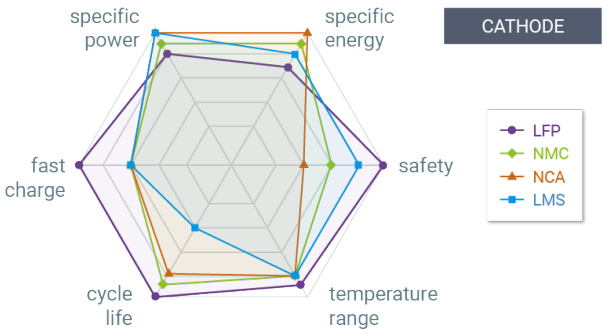


Article on Making Batteries Safer and Denser
Semiconductor Engineering Article

Addressing Alternative Technologies

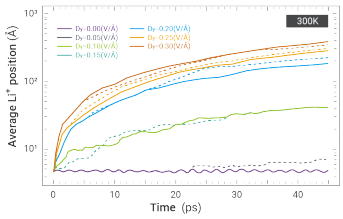
- Solid state batteries
- Solid / Polymer electrolytes
- Alternatives to Li-ion (Na, Mg, etc.)
- Li-S batteries
- Li-metal batteries
- Li-air batteries





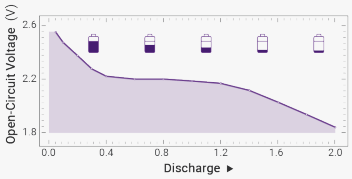
https://www.synopsys.com/silicon/quantumatk/materials-modeling/battery-simulation.html

QuantumATK Battery Material Modeling Application Examples



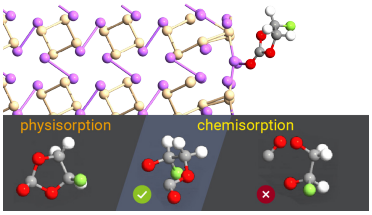
Li-ion Diffusivity in Cathode Under Electric Field

Gain deep understanding of Li-ion diffusion paths and mechanisms and screen materials with high Li-ion diffusivity and stable structures. In this example, Li-ion diffusivity (slope) is calculated in the $LiFePO_4$ cathode material using Molecular Dynamics (MD) with an external electric field which drives the diffusion at different temperatures and different electric field strengths. Benefit from the multi-model approach, that combines classical Force Fields (FF) with DFT, the latter to include the effect of the field and of time-dependent charge fluctuations.



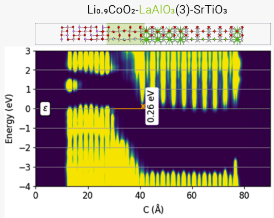
Open-Circuit Voltage Profiles

Obtain a profile of open circuit voltage (OCV) that indicates lithiation of a cathode during battery charge/discharge processes using molecular dynamics (MD) tools. Optimize these processes by screening cathode materials for morphological evolution, degradation, and failure. This example shows a calculated open-circuit voltage profile of a Li-S battery.



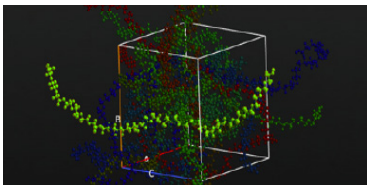
Formation of SEI at Anode Surfaces

Understand SEI formation mechanisms at anode surfaces to screen electrolytes and additives that help forming an initial SEI layer. This example shows how fluoroethylene carbonate (FEC) additive adsorbs on a lithiated Si anode surface and decomposes into different compounds depending on lithiated Si concentration and surface structure. Get insight into reaction paths and dominated interactions on realistic semi-infinite surfaces using the Surface NEGF method.



Interface Band Engineering

Calculate interface band offsets and band diagrams to screen interface materials for target interface electron conductivities for optimal battery performance. This example investigates if ultra-thin films, such as $LaAlO_3$, can be used for increasing electron conductivity at the cathode ($Li_{0.9}CoO_2$)/current collector ($SrTiO_3$) interface to improve the battery performance of the solid-state battery. Also, simulate the effect of thin films between anode and electrolytes to decrease electron conductivity for suppressing dendrite formation. Benefit from running DFT-LCAO calculations on large interface structures at a low computational cost.



Polymer Electrolyte Membranes

Investigate structural and electronic properties of polymer electrolytes. This example shows simulation of structure and electronic properties of poly(ethyleneoxide) (PEO) polymer. Benefit from automatic workflows for generating polymers and adding external ions or particles. Also, benefit from running DFT-LCAO calculations on large polymer structures (3500+ atoms), even with hybrid functionals such as HSE.

QuantumATK Advantages

Synergistic Solution

- Multi-level simulations to combine different engines in one workflow (e.g., combine Force Field and DFT)
- Ionic transport using advanced MD framework with hook functions (e.g., for electric field) and analysis tools
- Electron transport at interfaces with the NEGF-DFT method
- Surface NEGF for studying realistic complex surfaces without artificial finite size effects of the slab model

Realistic Physics of Complex Materials

- DFT-LCAO to simulate large systems at low computational cost
- Hybrid DFT functionals (HSE06, B3LYP, PBE0) for accurate formation energies and electronic structure
- Machine-Learning Force Fields for simulating Li-diffusion, automatic generation of training data

Effective Tools

- GUI workflows for generating complex structures, e.g., amorphous, liquids, nanostructures, interfaces, polymers, etc.
- Convenient analysis tools in GUI to extract the relevant quantities
- Convenient access to databases containing novel battery material structures (e.g., Materials Project)

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