Scientific Computing for Battery Research

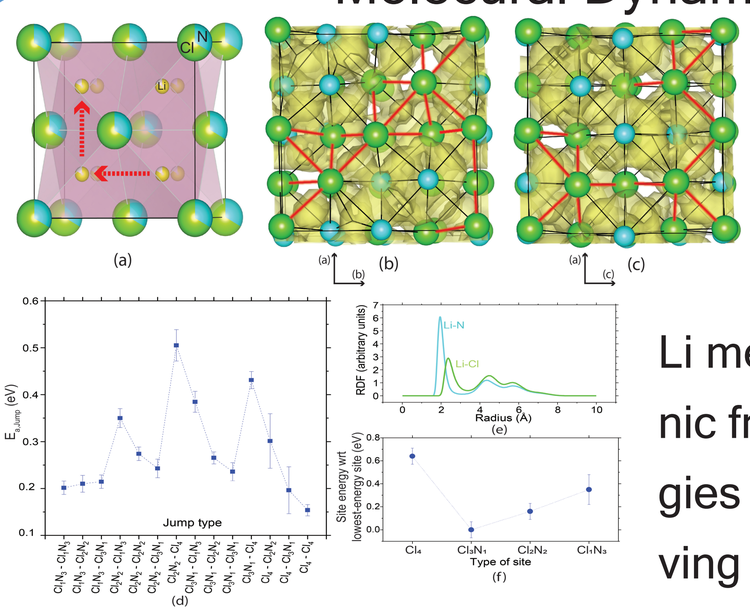
Towards a in-depth understanding and optimization

RST-Storage of Electrochemical Energy

SEE Group

In the SEE group we develop and study battery materials. The goal is to either understand better the current materails available or discover new ones towards new generations batteries.
To this end we use computational methods such as Molecular dyanamics simulations, both based on quantum calculations and force field methods. Morever Density Functional Theory is used to capture the behavior of active materials to model them in a phase-field based porous electrode theory.

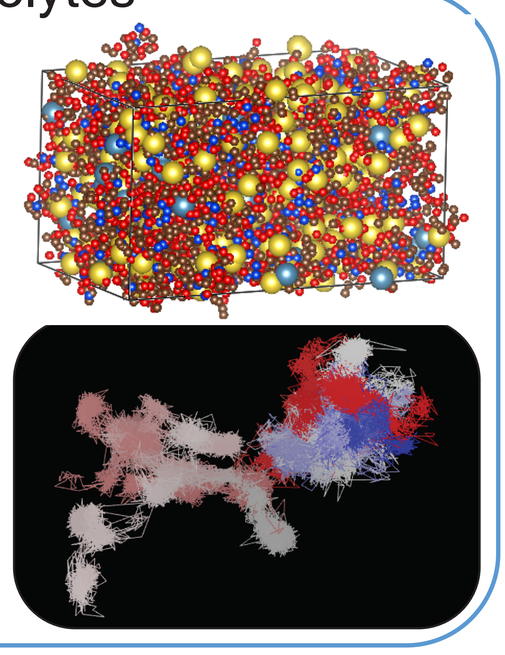
Molecural Dynamics of Solid Electrolytes



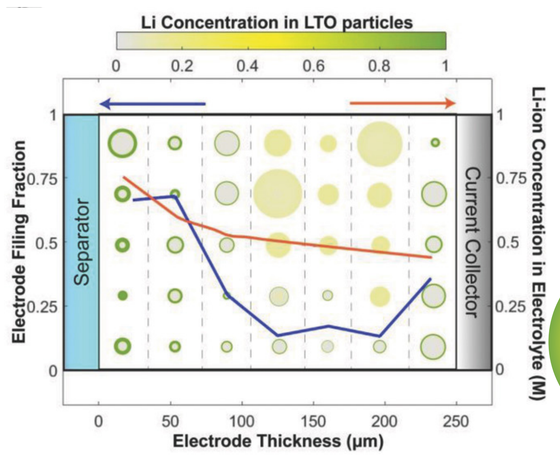
Molecular dynamics in solid electrolytes is a key technique to grasp the diffusion mechanisms. For example in Li_5NCl_2, one of the few compositions that is stable against Li metal, we found that due to disorder in the anionic framework a large manifold of migration energies exists in Li_5NCl_2 with some lithium jumps having much larger migration energies than others.

Molecural Dynamics of Liquid Electrolytes

Molecular dynamics calculations of alginate chains in the presence of different ions was done. We simulated 25 alginate chains of 12 monomers at room temperature with the gromos force field. The chains were cross-linked with calcium ions. A snapshot of this simulation is shown. Furthermore a plot of a trajectory of a sodium ion is shown after adding some water molecules colored according to time step from red via white to blue. Mobility was found higher for larger water content.

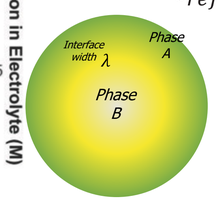


Multiphase Porous Electrode theory



$$G = \sum_{i=1}^{n}\left[\int kT(\tilde{c}_i\ln(\tilde{c}_i) + (1-\tilde{c}_i)\ln(1-\tilde{c}_i)) + \Omega_i\tilde{c}_i(1-\tilde{c}_i) + \tilde{c}_i\mu_i^{\Theta} + \frac{1}{2}\kappa_i|\nabla\tilde{c}_i|^2\right]$$

$$\mu_i = \frac{1}{c_{ref}}\frac{\delta G}{\delta\tilde{c}_i} = kT\ln\left(\frac{\tilde{c}_i}{1-\tilde{c}_i}\right) + \Omega_i(1-2\tilde{c}_i) + \mu_i^{\theta} - \kappa_i\nabla\tilde{c}_i$$



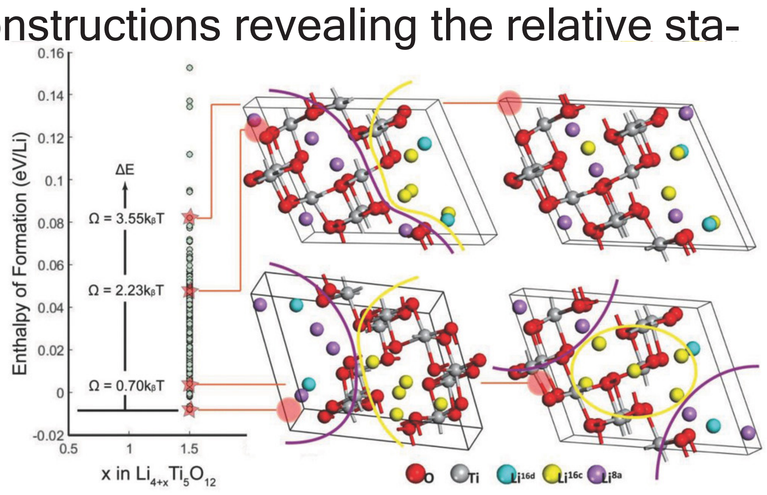
The application of phase-field methods to the porous electrode theory leads to a deeper undertanding of phase transitons inside the active materials of a battery. Here is an example of application on LTO, a popular anode with fast charging capabilities and long cycle life.

Delft Blue

The SEE group will extensively utilize Delft Blue to investigate the nanoscale properties of batteries and other energy-related materials. Our prime goal is to unravel relevant materials' core thermodynamic, kinetic, and structural properties for next-generation applications. We hope to use Delft Blue to undertake challenging AIMD simulations of size-significant and complex systems, including interfaces, coatings, and high-entropy mixing. More specifically, DFT-machine learning-driven molecular dynamic simulations will be at the center of our interest.

Interaction Energies in Battery Active Materials

Phase field models require fundamental thermodynamic and kinetic parameters as inputs. We investigate convex hull constructions revealing the relative stability between phases. In this example, we quantify the mixing penalty of the LTO phase separating in Li-rich and Li-poor regions within its subnanometer crystal lattice. We obtain the otherwise fitted parameters by measuring the energy difference of the stable phase-separated phase and complete mixing.



TU Delft

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