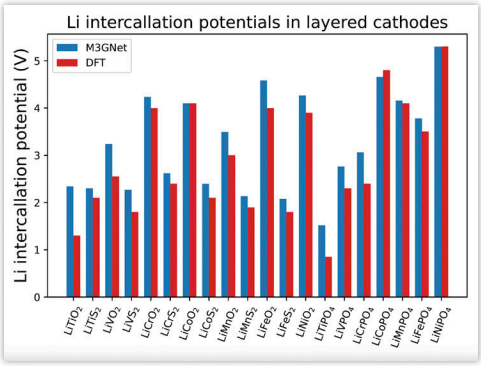
# Batteries
## with the Amsterdam Modeling Suite

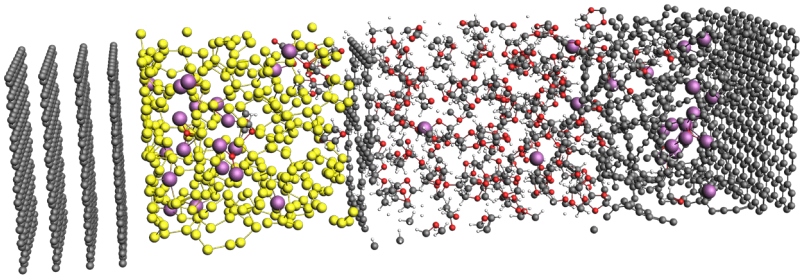
### Understand mechanisms and processes, at the atomic scale

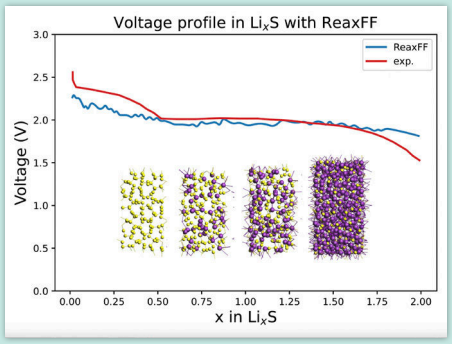
Accelerate R&D to reduce cost and environmental impact, improve lifetime and battery safety. From fundamental molecular properties to large scale reactive simulations of interfaces with explicit electrons, model and optimize electrodes, electrolytes, and interfaces.




### What can you compute with AMS?

- Intercalation potentials
- Voltage profiles
- Diffusion coefficients
- Charge mobility
- Phase diagrams
- Redox potentials
- Viscosity



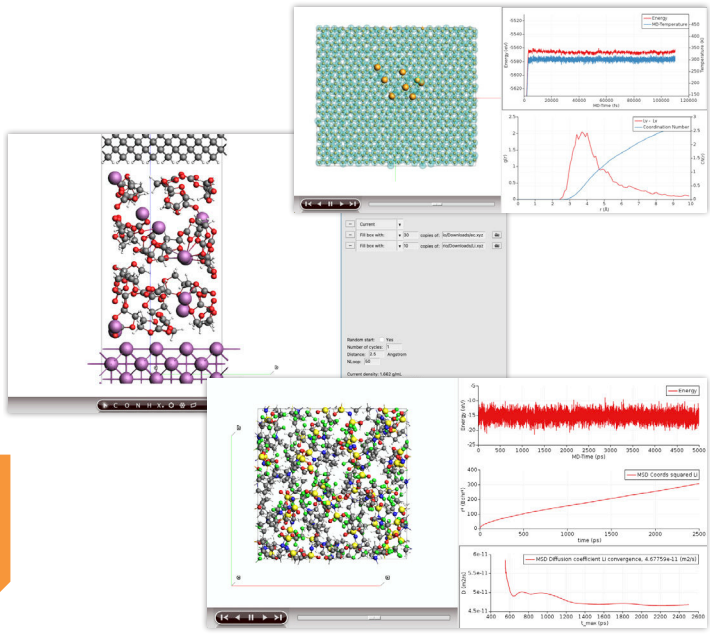



### Key methods for battery modeling

- √ Grand-Canonical Monte Carlo
- √ ReaxFF, eReaxFF, Machine Learning Potentials, Apple&P
- √ Nudged elastic band, PES scan
- √ Kinetic Monte Carlo to study kinetics
- √ DFT and COSMO-RS for redox potentials & solubility

### Tools and analysis for battery modeling

- Molecular builder
- Interactive molecular dynamics analysis
- Automatically extract reaction paths and rates
- Plot density profiles
- Automatic PES exploration and binding



SCM
Software for Chemistry & Materials

Explore batteries with AMS

# Batteries

## with the Amsterdam Modeling Suite

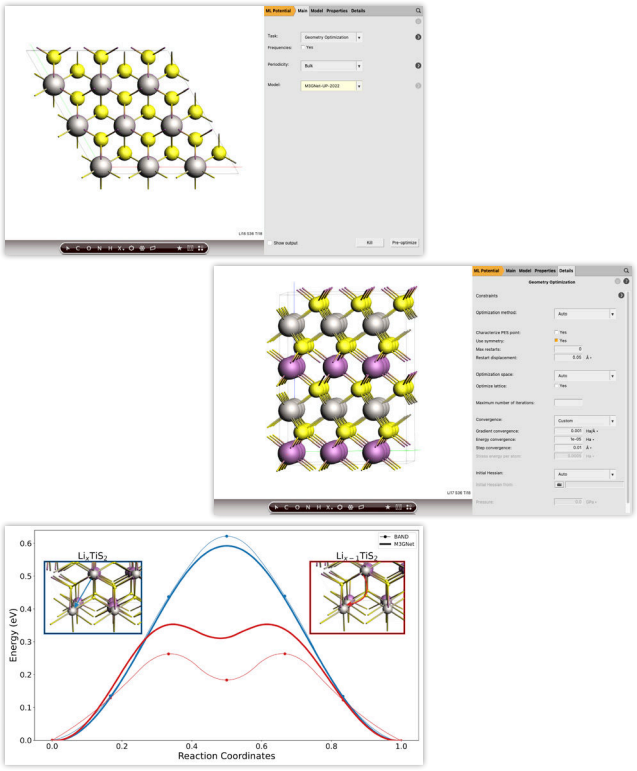
SCM
Software for Chemistry & Materials

### Li diffusion in $LiTiS_2$

In some Li-based cathode materials, the diffusion of Li ions is tightly connected to the content of Li atoms in the materials. We demonstrate this with atomistic simulations by computing the diffusion barrier of Li in $LiTiS_2$ with 1 and 2 Li vacancies. In layered $LiTiS_2$, the lithium ions are octahedrally coordinated between the S–Ti–S sandwich layers.

### Methods and results

To evaluate the diffusion of Li ions, we computed the reaction pathway of Li from one octahedral site to another empty neighboring site with nudged elastic band (NEB). Setting up the NEB is straightforward with the graphical user interface. We compared the universal machine learning potential M3GNet with the periodic DFT engine BAND. The resulting activation energies with M3GNet are accurate and comparable with those computed with BAND.




*"What I really like about the Amsterdam Modeling Suite is that the programs were clearly written by chemists for dealing with real chemical problems. A great suite of programs!"*

– Roald Hoffmann, Nobel Laureate

### About SCM

Scientists at SCM are passionate about making computational chemistry work for you. Our mission is to develop powerful, easy-to-use software for your research and development needs. We love to discuss your research and learn how we can serve you better in the future.

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