# Topological Analysis for Molecular Dynamics

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## *The performance of Lithium ion batteries is strongly influenced by the solvation and diffusion of the Lithium (Li) ion*

- Li-ion batteries are widely used in consumer electronics as well as large machinery
- How Lithium solvates and diffuses through the given electrolyte is still not well understood
- Of great interest are the reconnection events where the solvation structure of Li changes

## *First-principles molecular dynamics simulations can be used to model the solvation behavior from quantum-mechanical interactions*

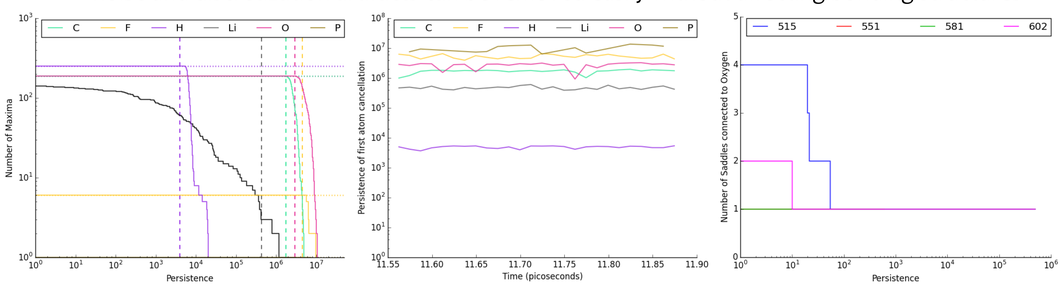
- Such simulations are computationally expensive, typically performed only for a few hundred atoms on time-scales of only tens of picoseconds
- A large computational effort yields a very small number of events of interest, slowing down the understanding of the process

## *Scalar field topology can help exploring such large-scale data*

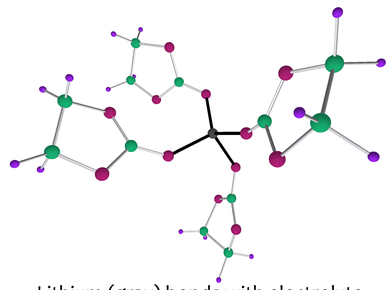
- The topology of the electron charge density (ECD) can be used to detect bonds [Bader, 1994]
  - atoms appear as local maxima in the function
- We compute the Morse-Smale complex of the ECD field, which captures its gradient behavior
  - two atoms are considered bonded if they are connected in the MSC
- Data can be explored efficiently this way, and various topological and geometrical properties become trivial to identify and track

## *Detection of bonds in a parameter-free manner*

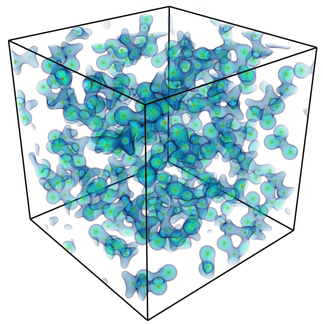
- Distance-based bonds are very parameter-sensitive and can lead to spurious reconnections events
  - requires a priori knowledge; atomic distances can change with temperature and pressure
- Topological-bonds are effectively parameter-free
  - noise and discretization artifacts can be removed easily without affecting bonding structures




- Topological definition of bonds are likely to be more reliable, especially during reconnections, which are unstable in nature



Lithium (gray) bonds with electrolyte molecules.

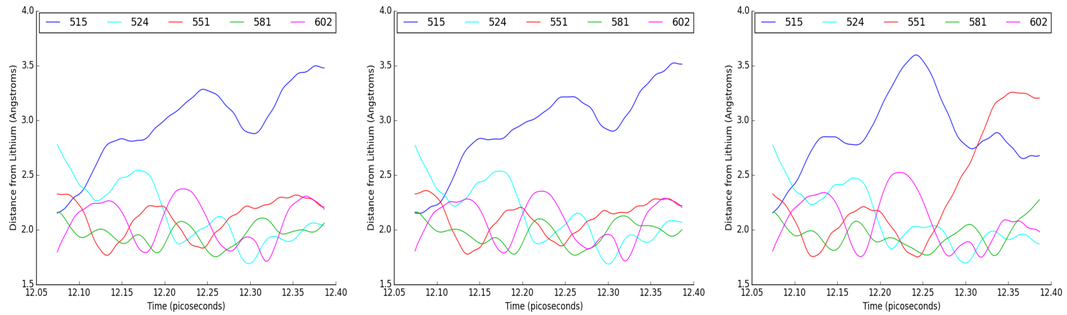


The electron charge density gives the relative probability of finding an electron at a given position.

## *Exploration of multiple simulation paths*

- By identifying unstable configurations in the simulations, we can create checkpoints and change simulation parameters to create new branches
- We may want to create, prevent, or delay a reconnection

- This still-exploratory study can help creating a larger number of reconnection events of interest
- This study can also provide a stability analysis for the underlying physical model with respect to the simulation parameters

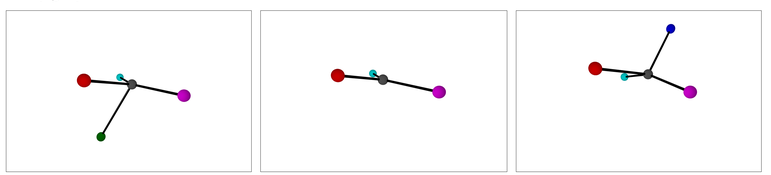



Two attempts (middle and right) to change the simulation future as compared to the original (left) 4-5-4 reconnection.

## *Detection and prediction of reconnection events*

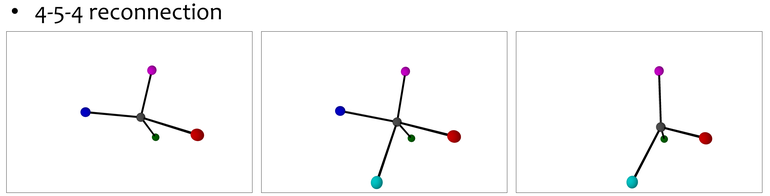
- Topological properties can indicate and predict a reconnection (an unstable configuration)

- 4-3-4 reconnection

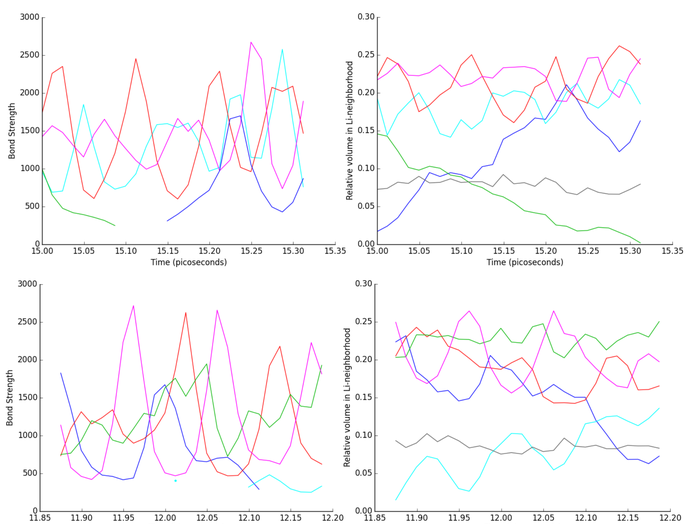


Lithium (gray) detaches itself from the green oxygen, and exists in an unstable configuration before attaching to the blue oxygen.

- 4-5-4 reconnection



Lithium (gray) gains a bond with cyan oxygen, creating an unstable configuration, causing it to shed the blue oxygen.




This work was performed under the auspices of the US Department of Energy (DOE) by Lawrence Livermore National Laboratory (LLNL) under contract DE-AC52-07NA27344. LLNL-POST-673375.