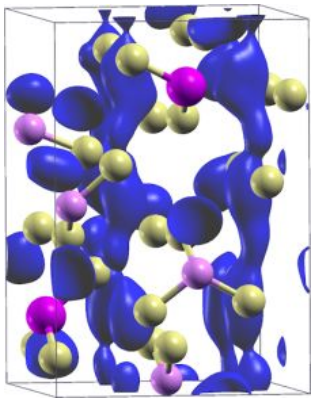
Connecting Scales: Learning Dynamics for Efficient Ionic Conductivity Predictions with Graphs

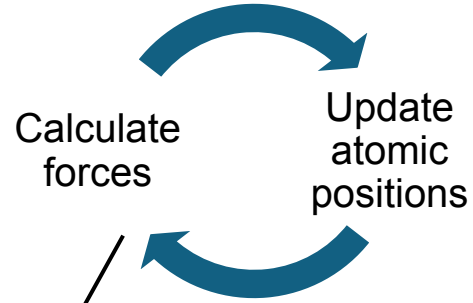
Why superionic solids

- Improved safety
- High gravimetric and volumetric energy densities



Materzanini, G., Chiarotti, T. & Marzari, N. Solids that are also liquids: elastic tensors of superionic materials. npj Comput Mater 9, 10 (2023). https://doi.org/10.1038/s41524-022-00948-8

Molecular Dynamics

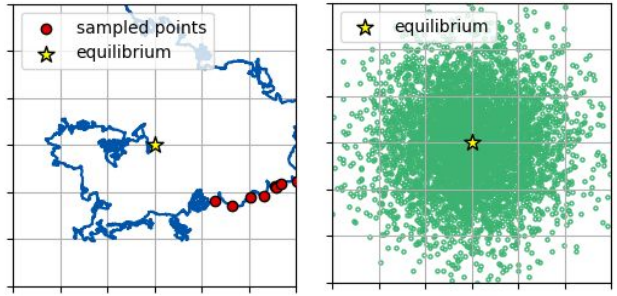


- Ab initio, DFT forces (AIMD)
- or ML force-fields

It takes weeks to simulate one material with DFT on a cluster

Alternative

- The first few steps of MD trajectory carry enough information.
- Random perturbations as the way to explore the energy landscape.



Results