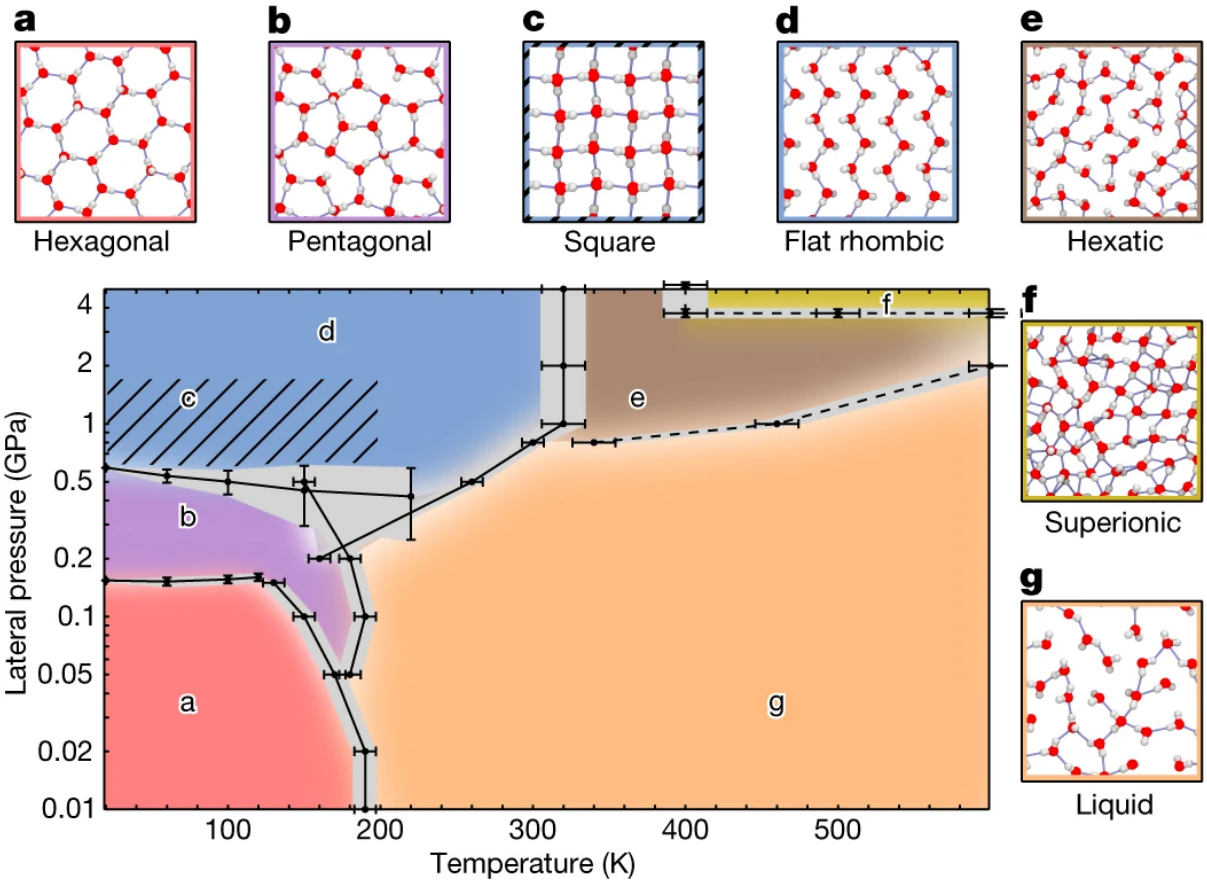
Hands-on 6. MD simulation analysis

What do we analyze in Molecular dynamics (MD)?

Few analystic/statistical approaches in MD field

▼ How we get statistically meaningful results?

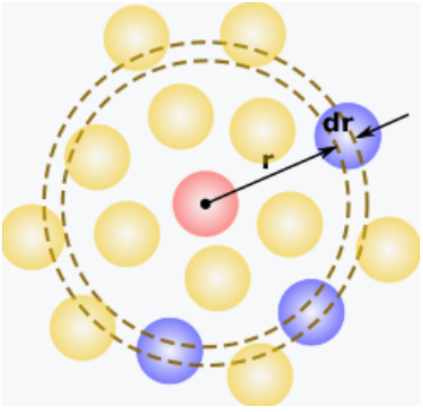
- Optimized water structure

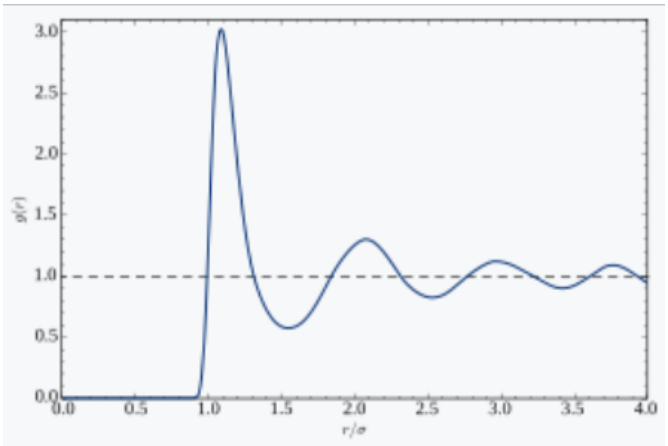


https://www.nature.com/articles/s41586-022-05036-x/

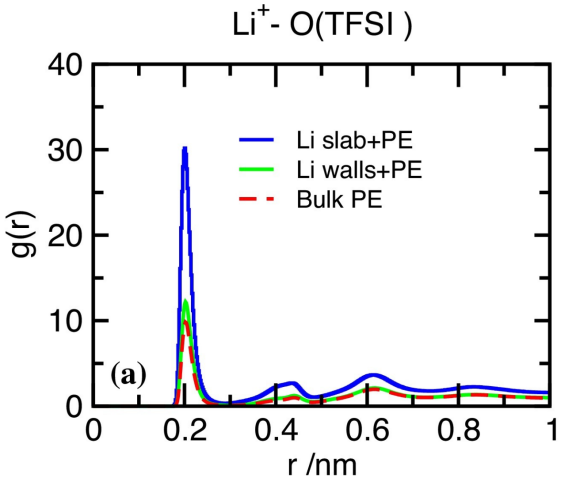
▼ How we check the distribution of my system: RDF

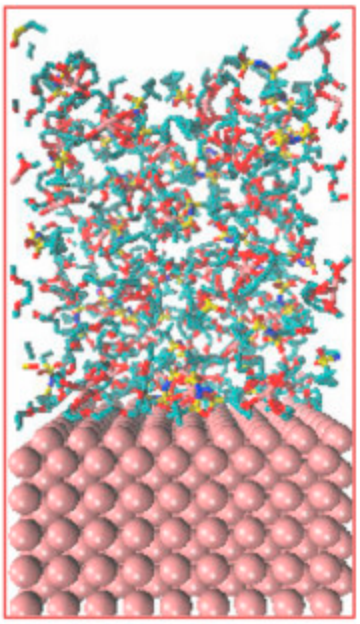
Radial distribution function (RDF)





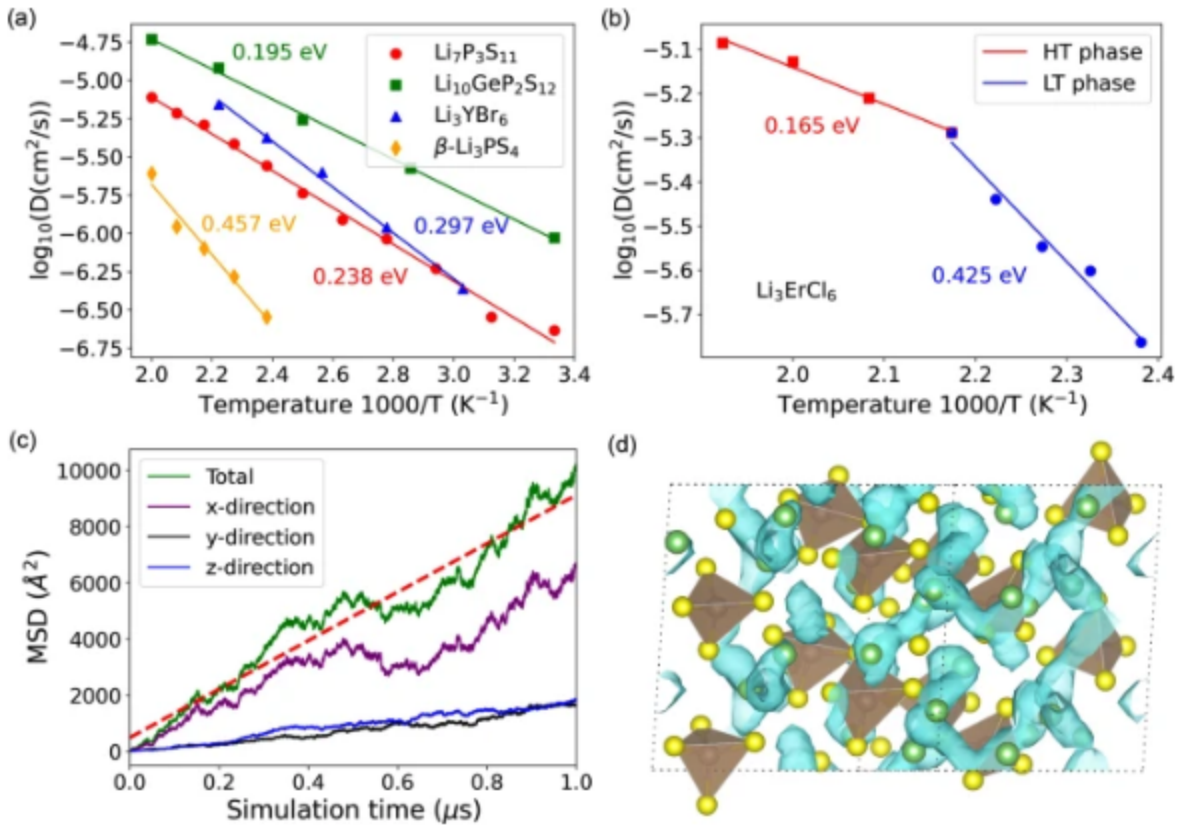
the **radial distribution function** , (or **pair correlation function**) g(r) in a system of particles (atoms, molecules, colloids, etc.), describes how density varies as a function of distance from a reference particle.





▼ How we monitor chemical reaction during MD?: MSD

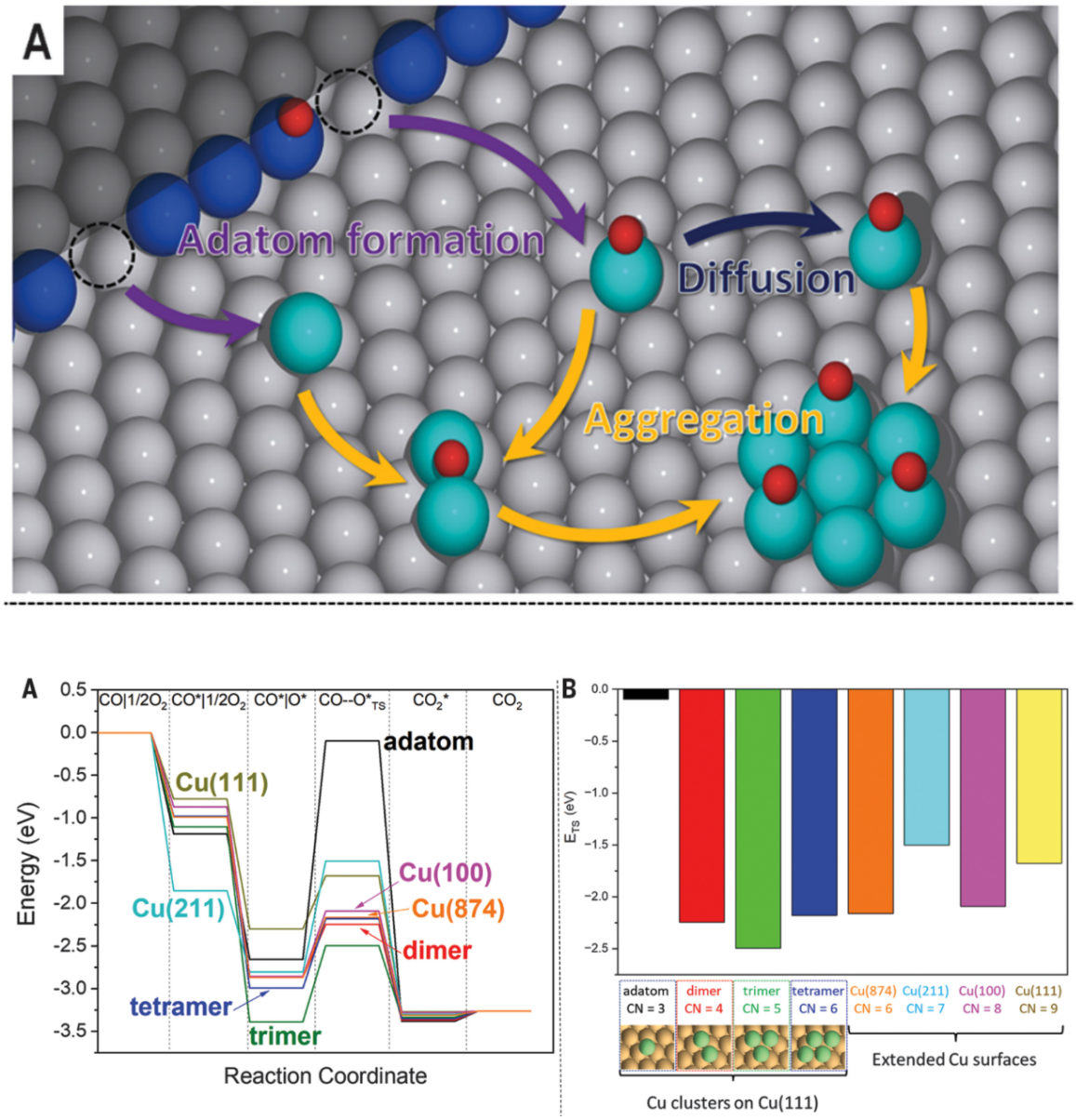
Li diffusion in solid state electrolyte



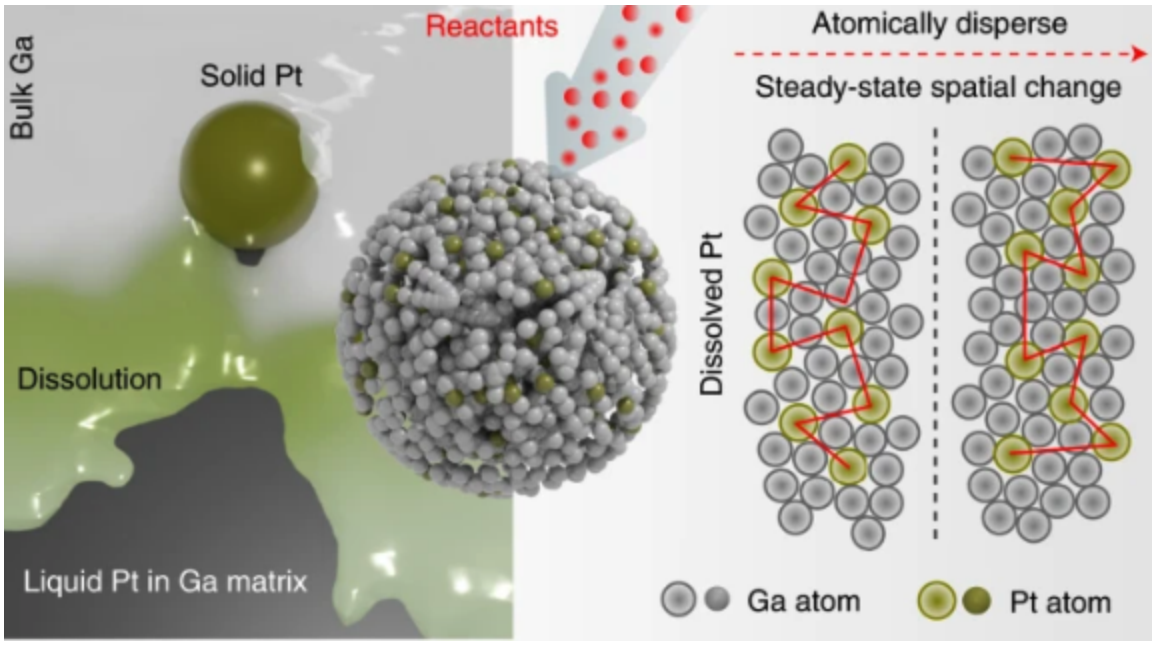
Task: Atomic diffusion of metal adatom

Simulation system:

transfer of metal atom.



https://www.science.org/doi/full/10.1126/science.add0089



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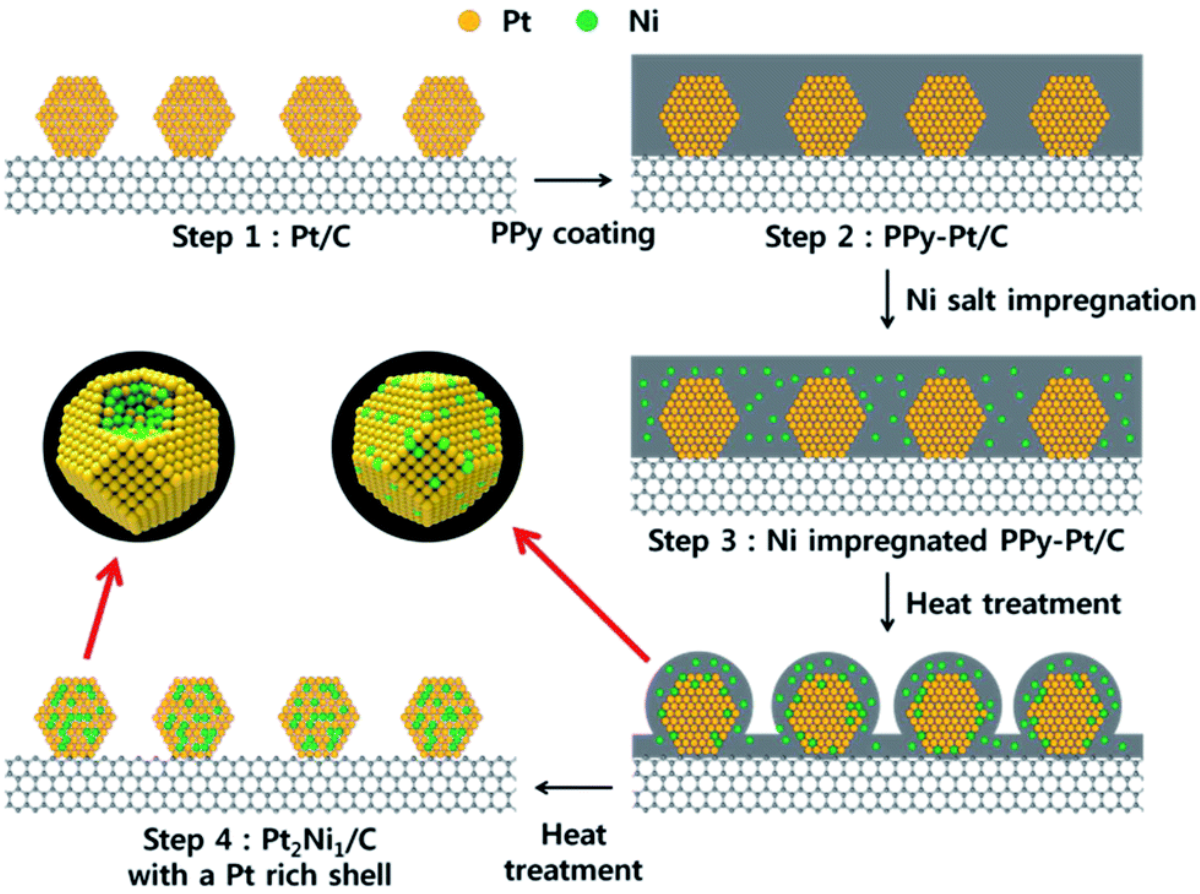
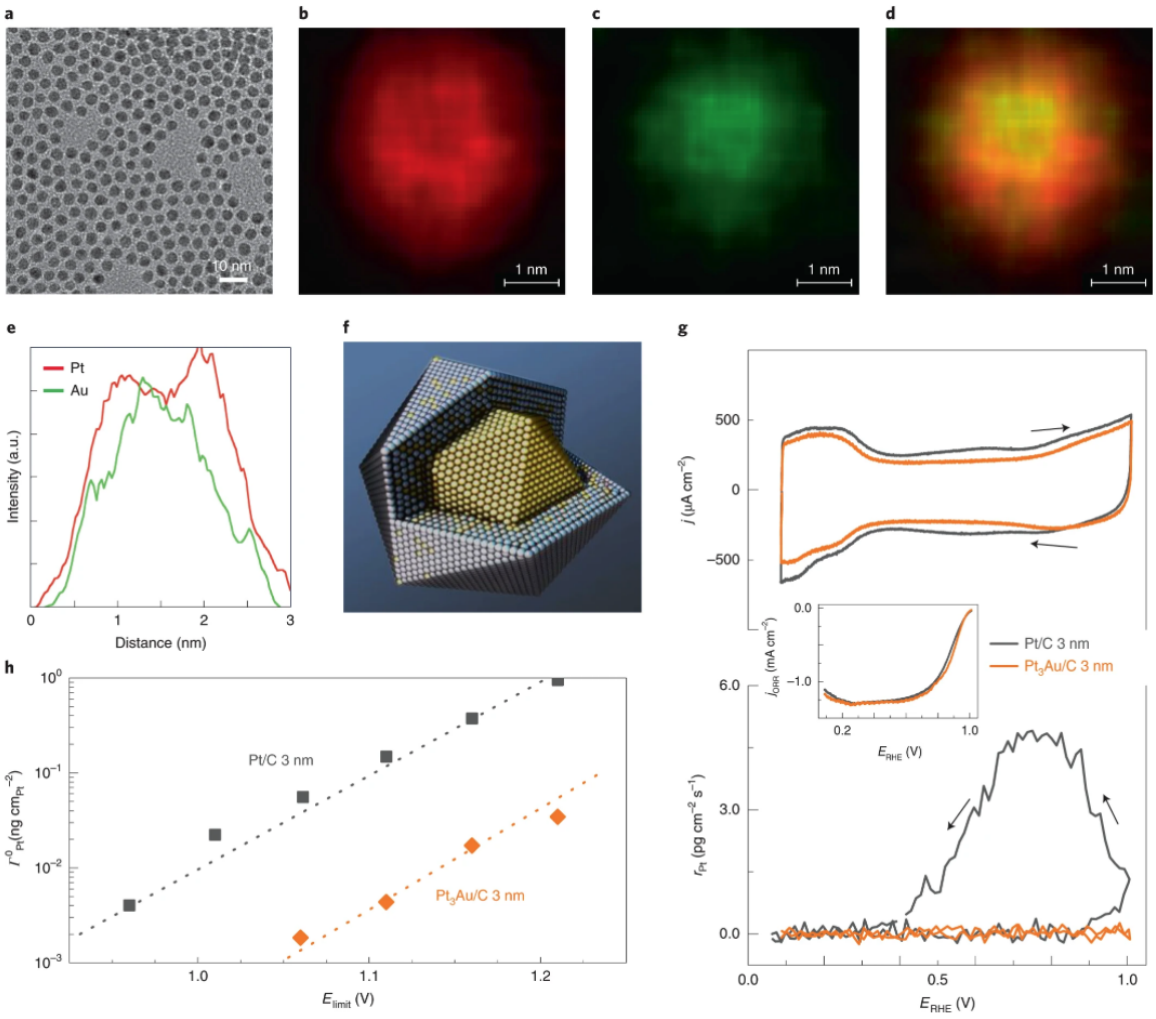


https://pubs.rsc.org/en/content/articlelanding/2014/ta/c4ta01328j



https://www.nature.com/articles/s41563-020-0735-3/figures/4

Assignment

- **Choose two metal elements** from the following list: **Al, Cu, Ag, Au, Ni, Pd, or Pt**. (AVOID Pt/Au combination as same as tutorial)
- **Create a (111) facet slab** using the first selected element (e.g., Pt(111)).
- **Randomly place 10 atoms of the second selected element** on top of the (111) slab.
- **Run NVT molecular dynamics simulations** for at least 100 ps (constant Number of atoms, Temperature, and Volume) three times at **different**

temperatures.

- **Plot the Mean Square Displacement (MSD)** over time for the system and analyze the time evolution of MSD.