

MACHINE LEARNING OF ATOMIC DYNAMICS AND STATISTICAL SURFACE IDENTITIES IN GOLD NANOPARTICLES

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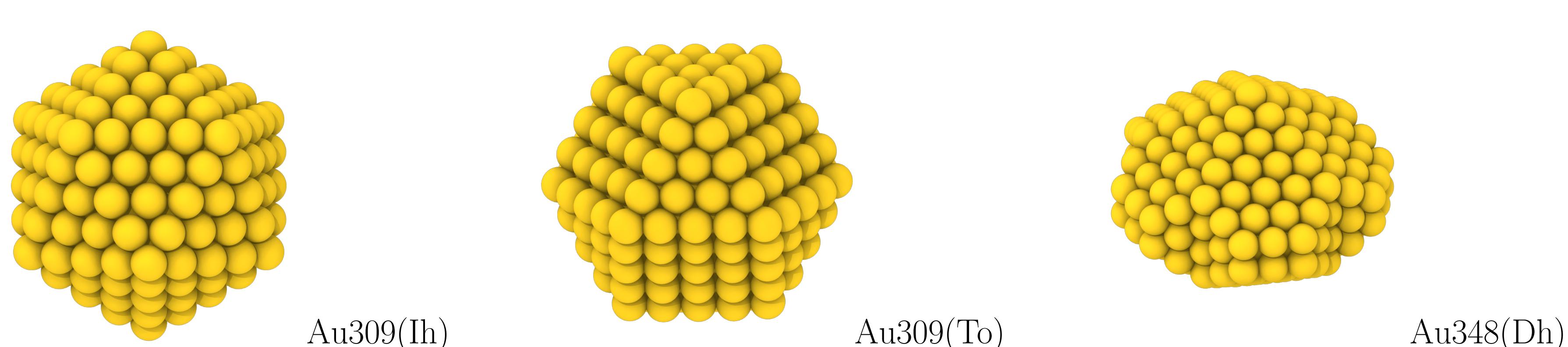
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Introduction

Our general **data-driven** approach allows for resolving complex dynamics within metal nanoparticles. We focus on gold NPs as a relevant example, but the approach is versatile and applicable to other systems. We simulate various types of Au NPs (*i.e.*, icosahedral, decahedral, octahedral) on relevant spatiotemporal scales. A combination of SOAP-based data-driven analyses reveals the **atomic environments** populating Au NPs along the MD simulations at various temperatures.

Systems

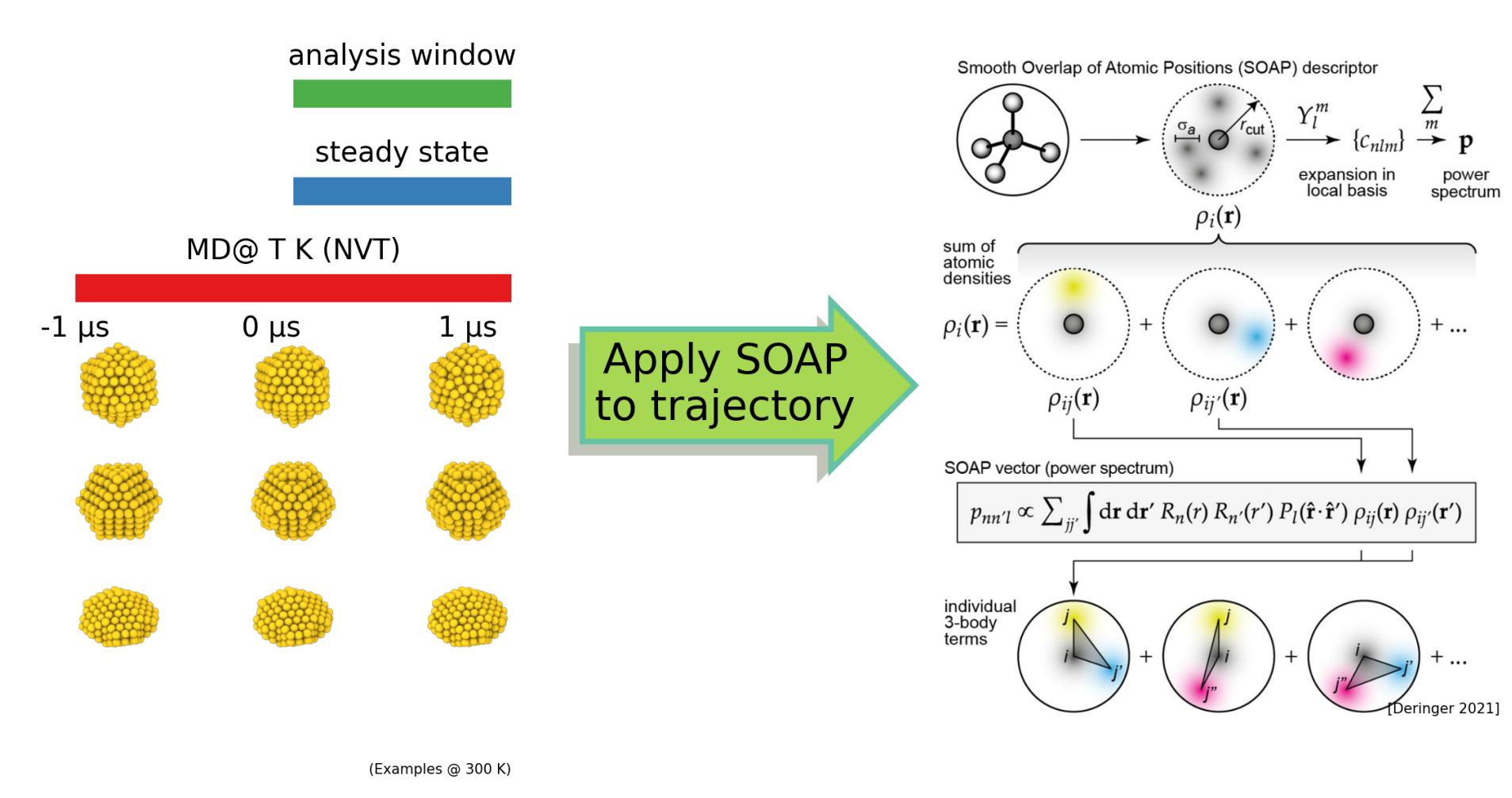


Software

- Python
- dscribe
- HDBSCAN
- scikit-learn
- scipy
- SOAPify

See also:
Cioni *et al.*:
arXiv:2207.14622
Rapetti *et al.*:
10.26434/chemrxiv-2022-7wfm9-v2

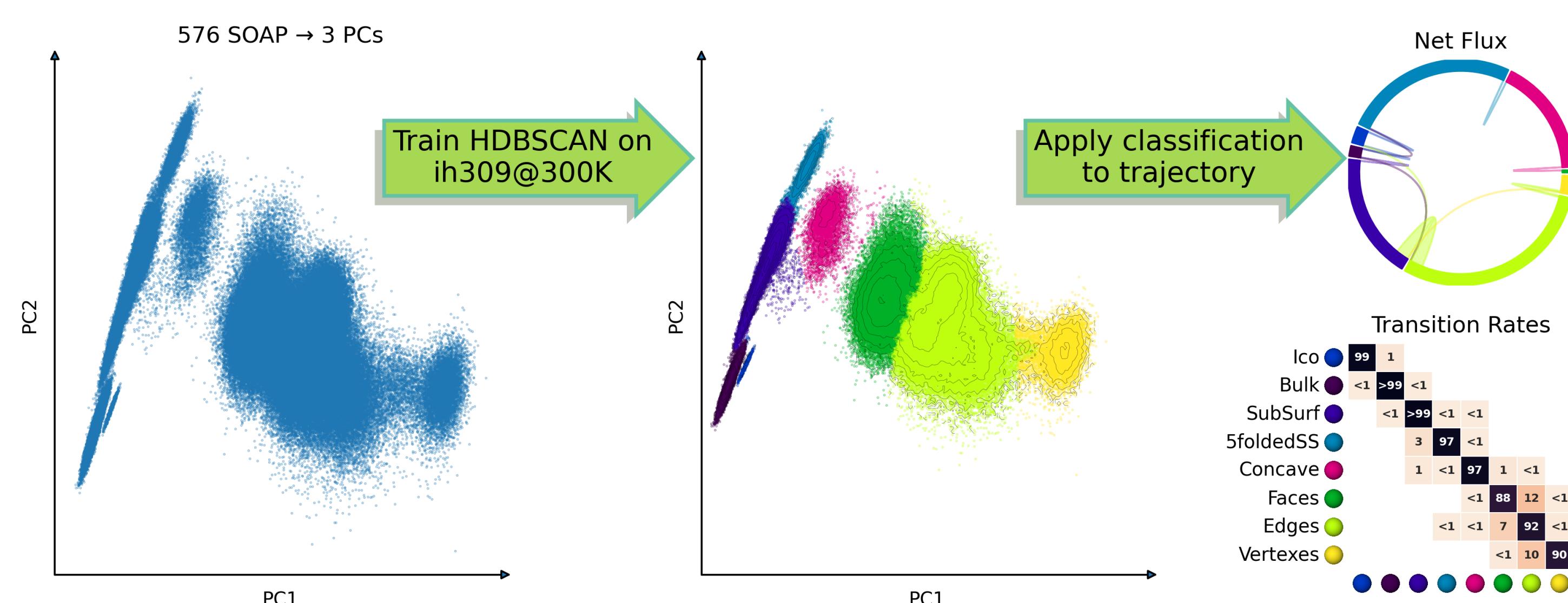
From Simulation to SOAP Fingerprints



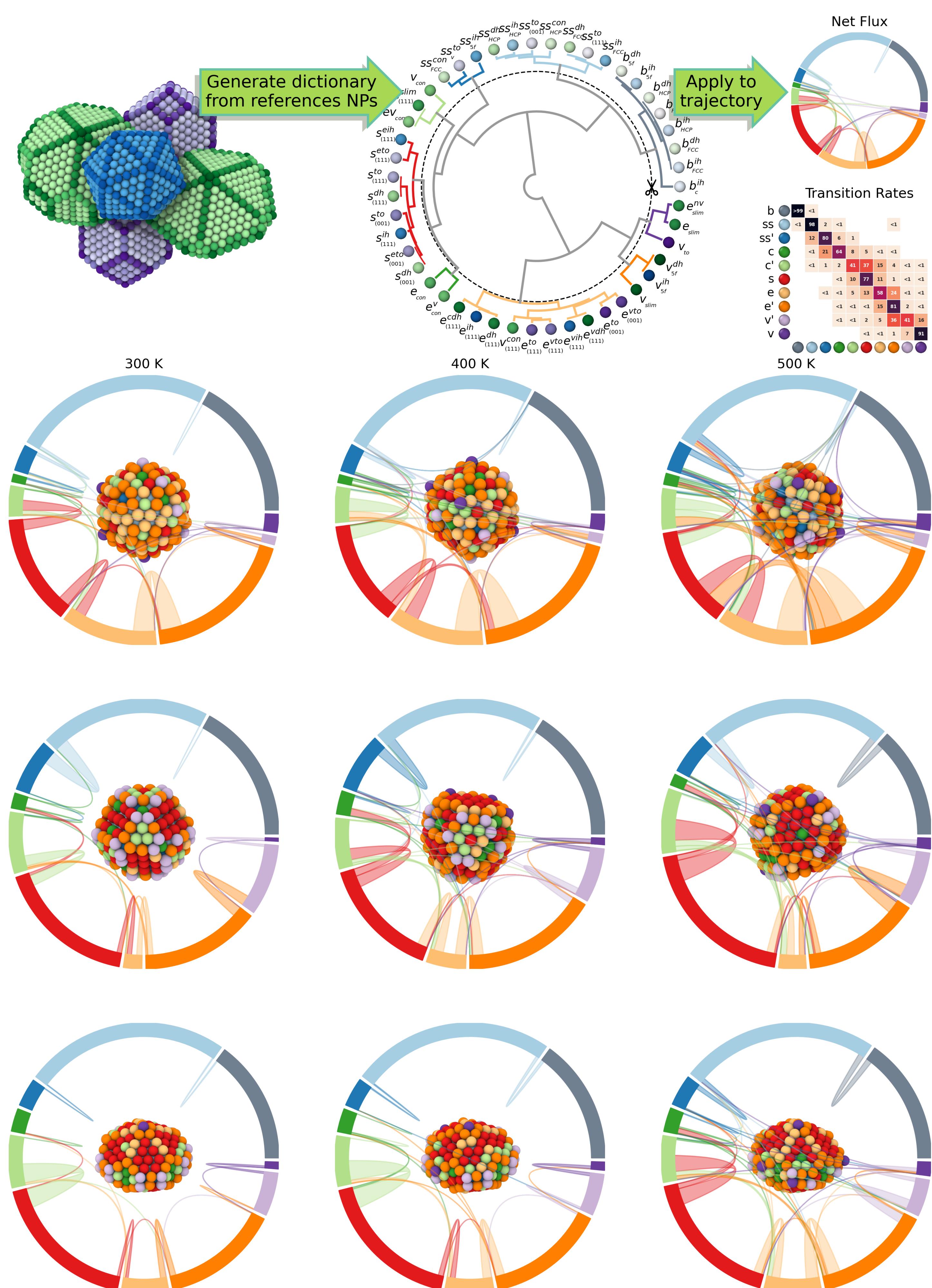
Animations



Bottom Up



Top Down



Acknowledgements

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Perspectives

- Apply procedure to alloyed and oxidized materials
- Apply procedure to material in **active** environment
- Accurate determination of the **transition times**