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INAR Institute for Atmospheric and Earth System Research

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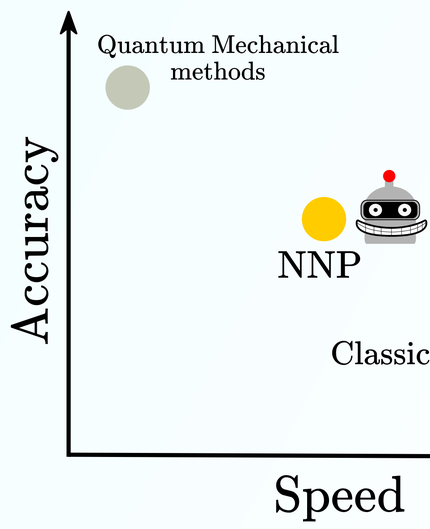
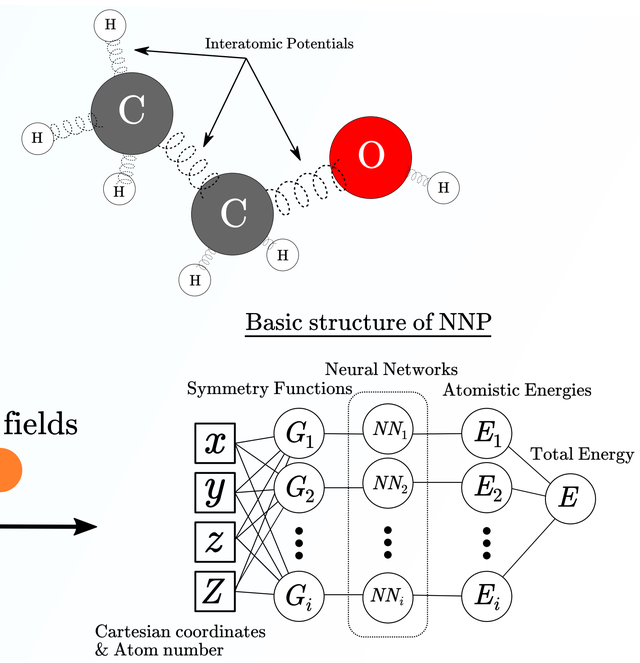
Using New Generation Neural Network Potentials to Benchmark Ice-Water Equilibria

WHY?

- Understanding the formation and growth of **ice and mixed phase clouds** in Earth's atmosphere is of great interest.
- **Cloud droplets** freeze heterogeneously on ice nucleating particles (**INPs**) at moderate supercooling.
- A **wide range of materials** can act as INPs, such as mineral dust, pollen or organic aerosol.
- **Modelling** the ice growth on the particles can be challenging, as creating **force fields** for indivudual ice-water-particle systems is **time consuming**.
- Neural Network Potentials (NNPs) are a solution this. So called **Foundation Models** are able to simulate such systems 'out of the box'.
- **But how good are they really?** Here we assess how accurately they predict **the melting point of ice.**

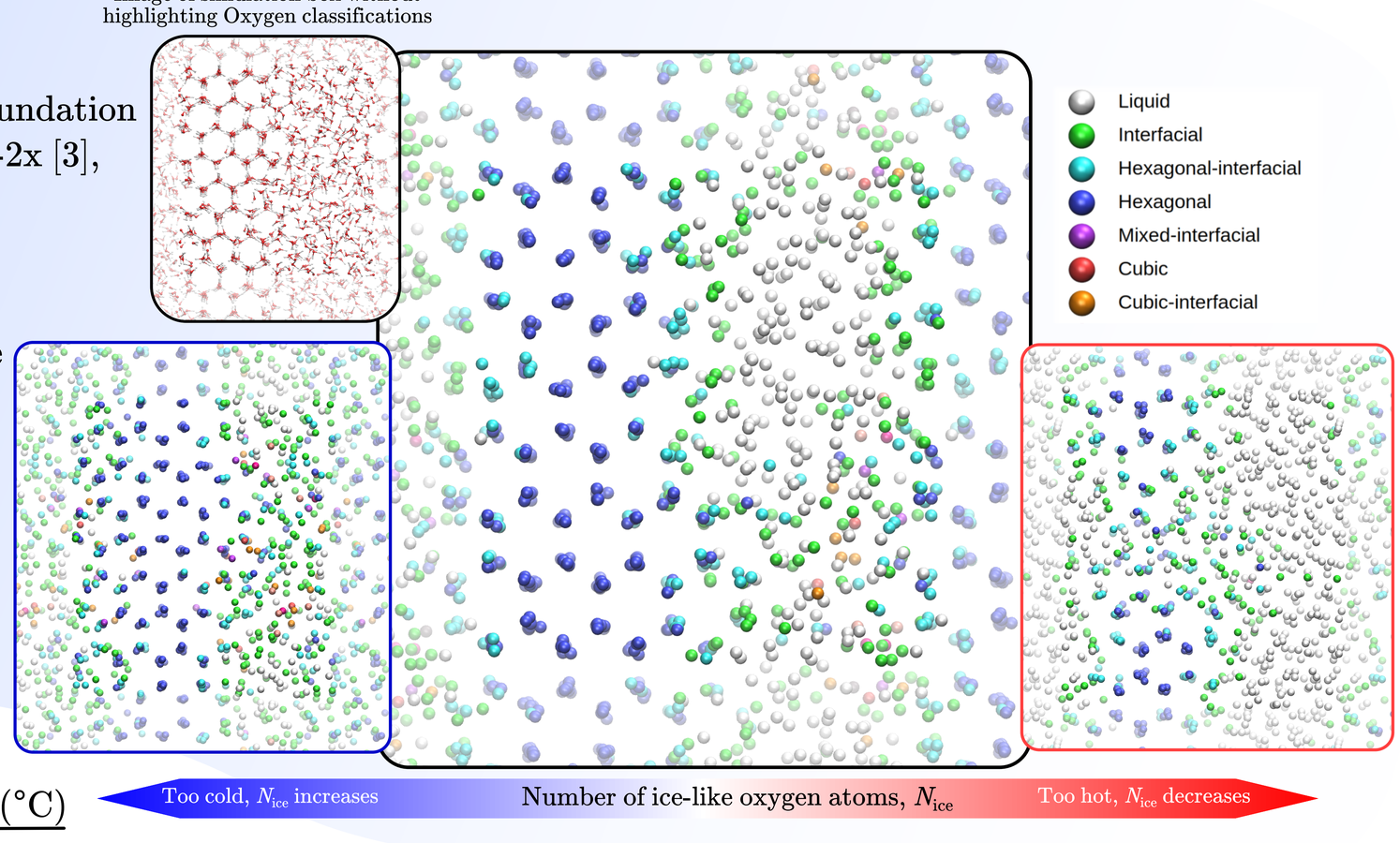




HOW?

- We have benchmarked the melting point of seven foundation models: SO3LR [1], MACE-MP [2], ANI-2dr & ANI-2x [3], Orb3 & Orbmol [4], and FENNIX-Bio1. [5]
- To find the melting point of water for these NNPs, we perform Molecular Dynamics (MD) simulations.
- We count the number of ice-like molecules over time using LICH-TEST [6] implemented in GPTA. [7]
- The temperature at which the number does not change is the melting point.
- Computational resources were provided by CSC, the Finnish IT-Centre for Science.

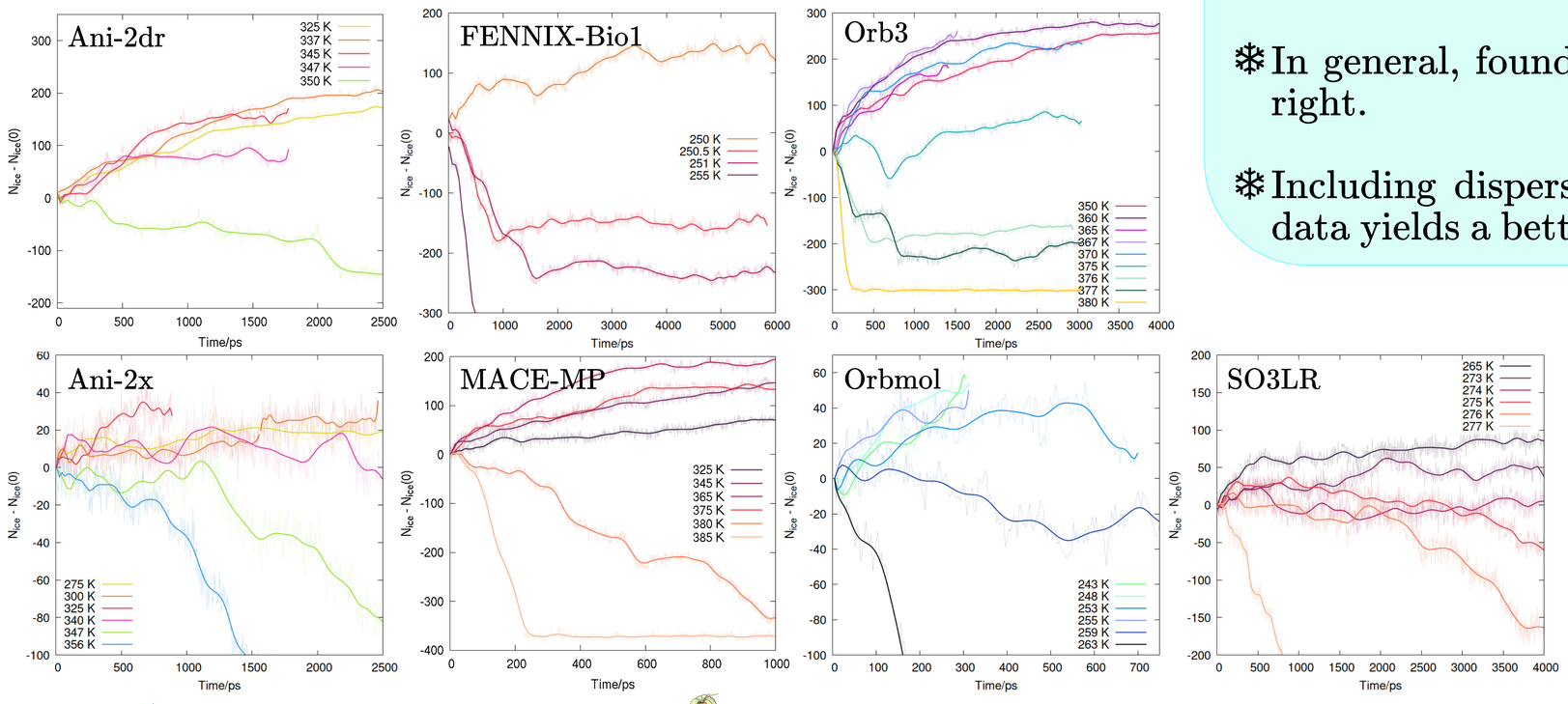
Image of simulation box without highlighting Oxygen classifications



RESULTS

* = Can be faster

NNP	Dispersion	Speed (ns/day)	Melting Point (°C)
ANI-2dr	Yes (No)	0.6	75
ANI-2x	No	1.3	67
FENNIX-Bio1	Yes	**4.1***	-23
MACE-MP	No	0.6*	104
Orb3	No	1.2	102
Orbmol	Yes	0.13	-15
SO3LR	Yes	2.9	**1**



SUMMARY

- There is limited availability of classical force fileds that can simulate INP relevant surfaces.
- Simulating atomistic trajectories at near quantum chemical accuracy is now possible with NNPs.
- In general, foundation models do not get the melting point right.
- Including dispersion and ice-like structures in the training data yields a better melting point.

[1] A. Kabylda et al., ChemRxiv (2025)
[2] I. Batatia et al., arXiv (2025)
[3] C. Devereux et al., J. Chem. Theory Comput. (2024)
[4] M. Neumann et al., arXiv (2024)
[5] T. Plé et al, ChemRxiv (2025)
[6] P. Raiteri, https://github.com/praiteri/GPTA
[7] G. Roudsari et al., J. Phys. Chem B (2021)

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