

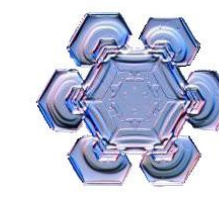
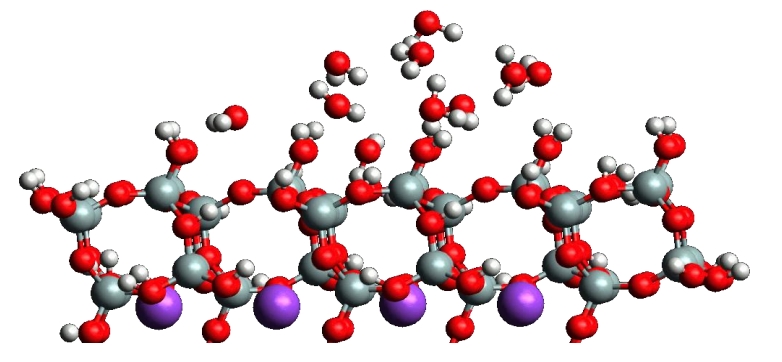
Ice Clouds and Ice Nucleation in Arctic

FROM ATOMS TO GLOBAL MODELS: SIMULATING CLOUDS IN THE ARCTIC

Ice nuclei (IN) affect the Arctic climate for example by controlling the cloud cover. Arctic area is depleted of IN / CCN, and therefore any changes in their abundance from changes of sea ice coverage, land use and pollution can have a clear effect in the Arctic.

Remote sensing observation analysed in ICINA indicate that both the type of aerosol (IN efficiency) and the amount of aerosol (CCN concentration) affect the cloud phase in the Arctic. To understand observations modelling efforts in different scales are needed.

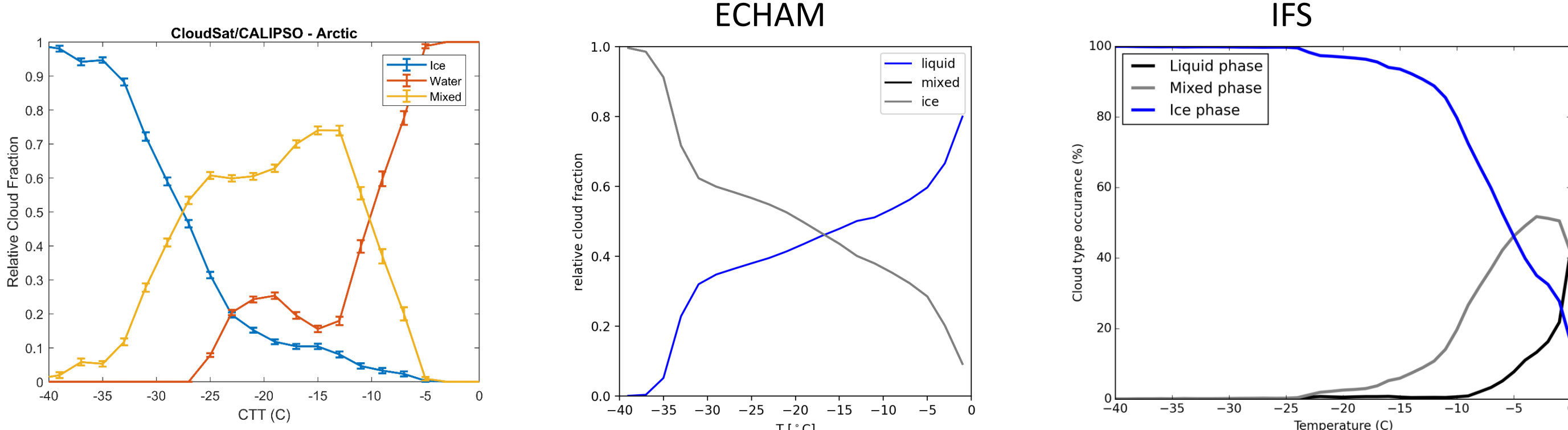
Simulation methods



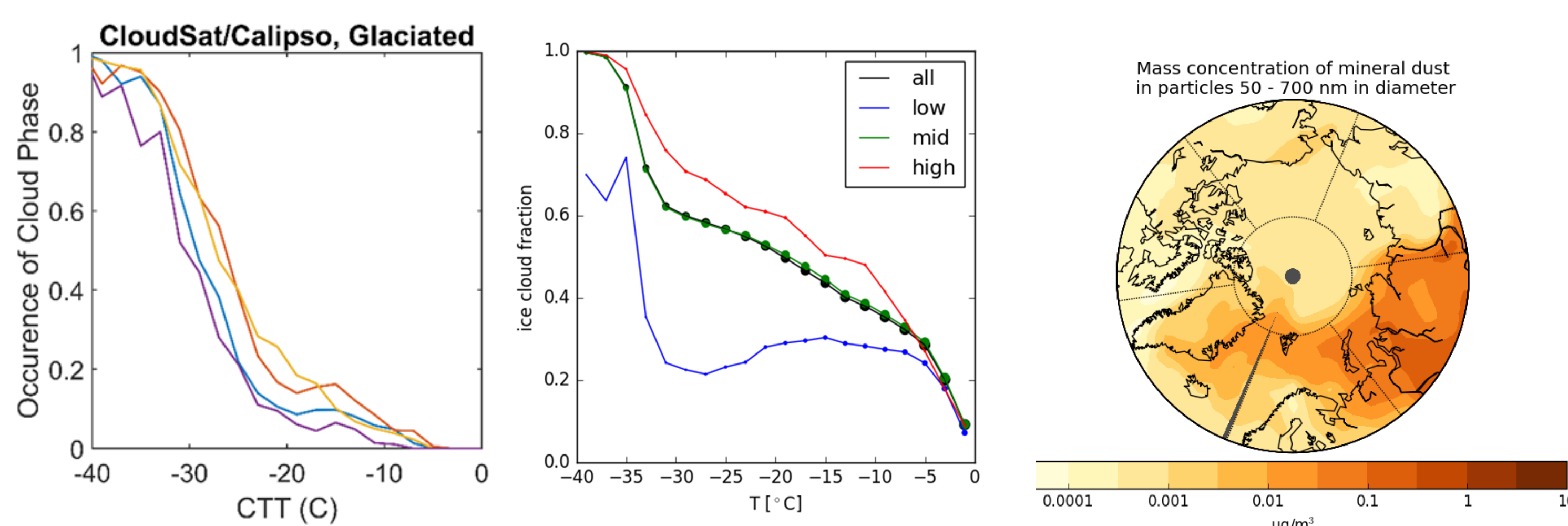
Molecular dynamics (MD) supported by DFT
UCLALES-SALSA cloud resolving model
with explicit aerosol-cloud interactions
Global atmospheric models ECHAM and IFS

Climate model

Different climate models and ICINA observations show highly different frequency of different cloud phases in the Arctic



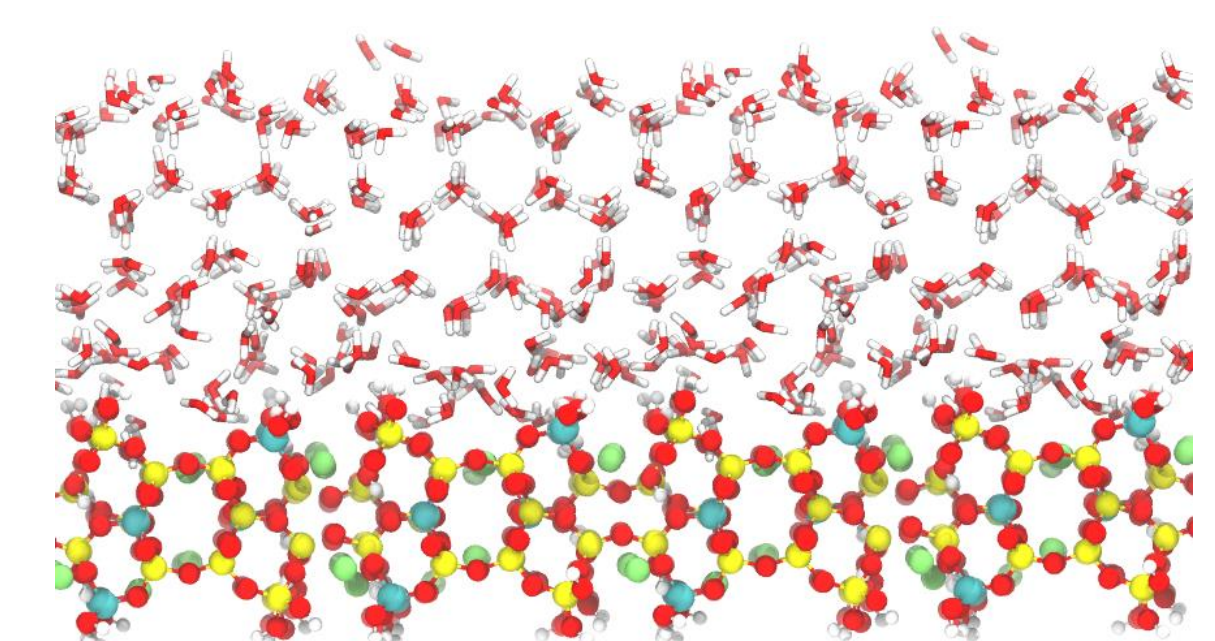
In ECHAM, cloud phase is dependent on DUST concentration.



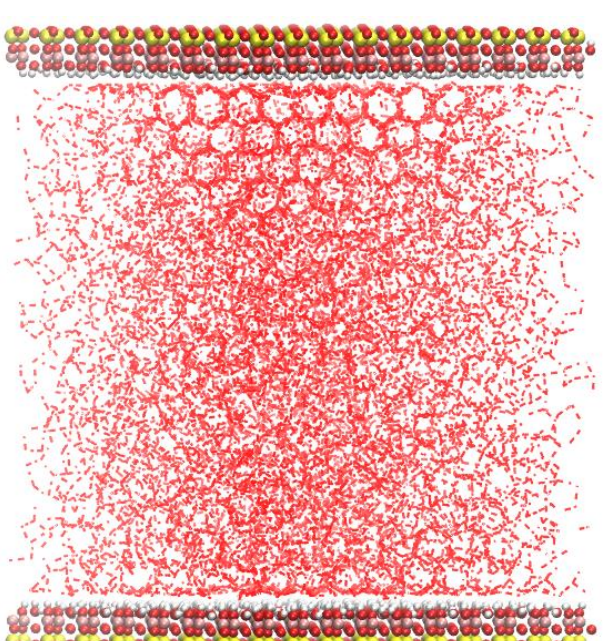
Molecular level simulations

There is a growing understanding of the role of surface topography on heterogeneous ice nucleation. Surface features such as pores, pits, cracks, steps and defects on surfaces function as **active sites**, where ice nucleation happens.

- Mineral dusts, specifically K-feldspars have been determined to be the dominating ice nucleating particles in the atmosphere
- Origin of their activity is still under debate



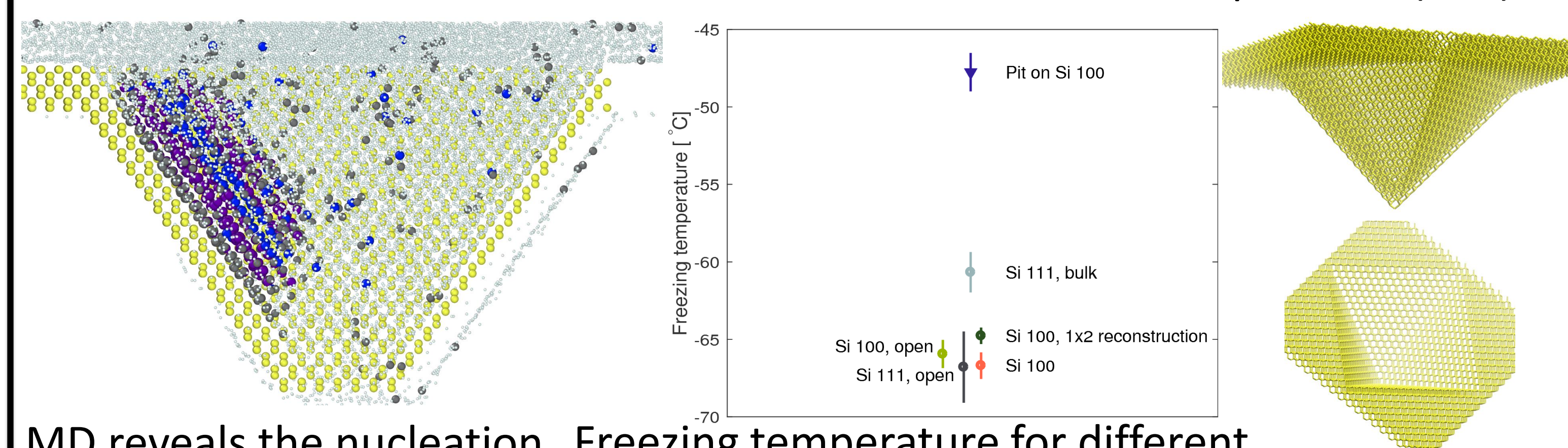
Feldspar microcline (100)
surface with ice at 243 K



Kaolinite is an effective ice
nucleating clay mineral

Direct comparison to experiment: topography

MD simulations of enhanced ice nucleation in KOH etched pits on Si(100)



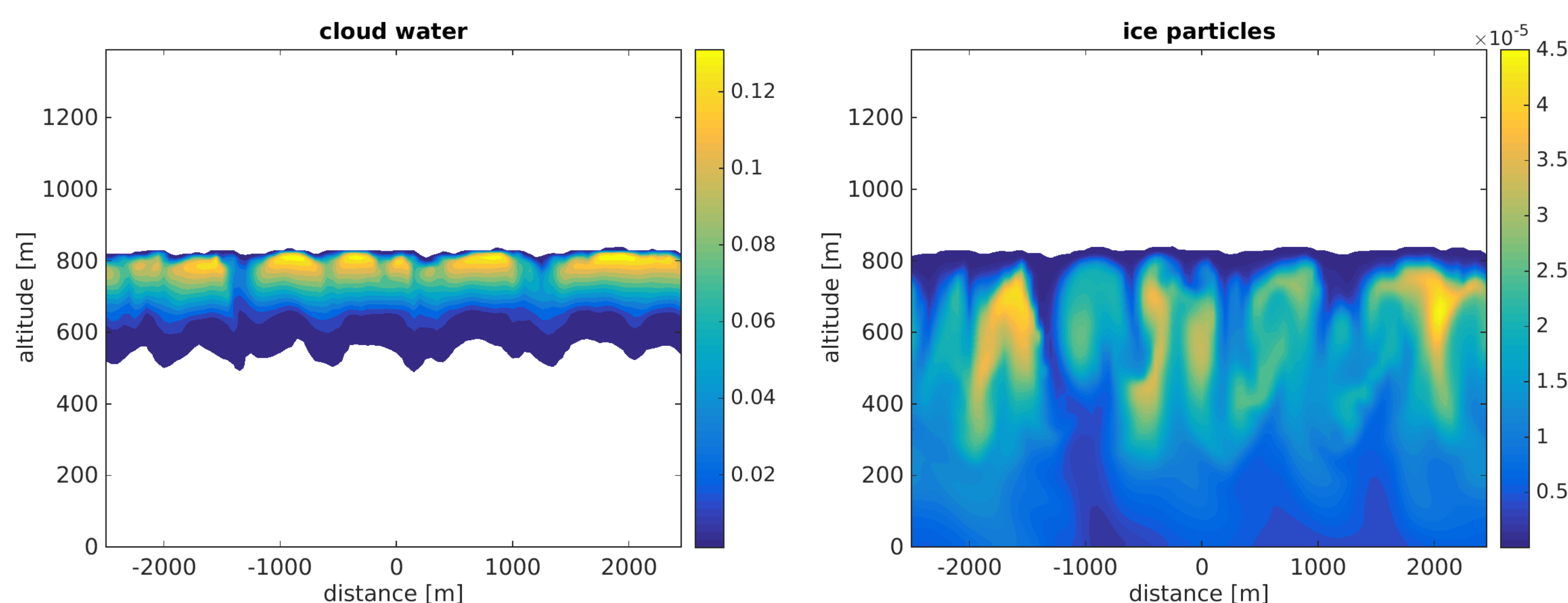
MD reveals the nucleation sites at atomic precision, showing nucleation and growth of ice inside pits.

Freezing temperature for different cells show a clear **12.9° C** increase in freezing temperature in a pit, compared to flat (111) surfaces.

Effect has been experimentally confirmed.

Cloud resolving simulations

In ICINA, UCLALES-SALSA cloud resolving model was updated to include aerosol particle – cloud droplet – ice particle – interactions.

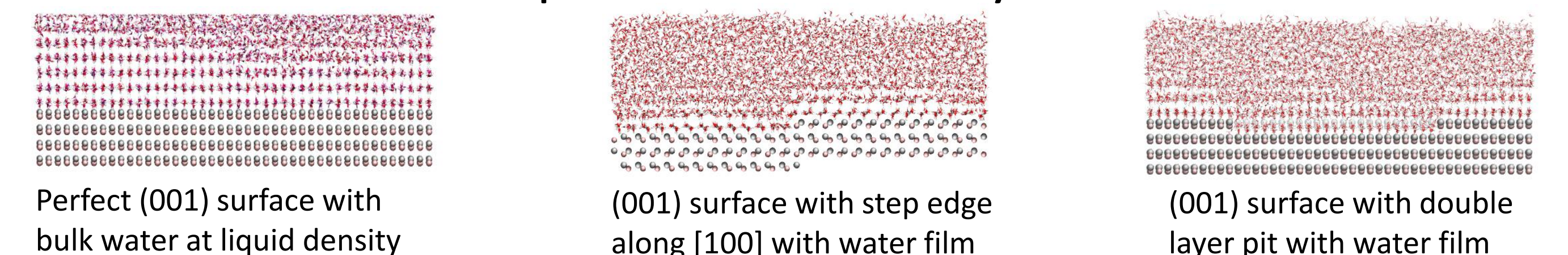


New tool was found highly skilled in simulating cloud properties. The results support observations on liquid topped mixed phase clouds with ice precipitation.

In pristine conditions increase in droplet concentration increases cloud lifetime due to enhanced radiative cooling and mixing, which delay ice particle formation and glaciation of cloud.

Silver iodide: effect of defects on nucleation

We have shown how activity of AgI is explained by its lattice match with ice. Examples from our study of the effect of defects:

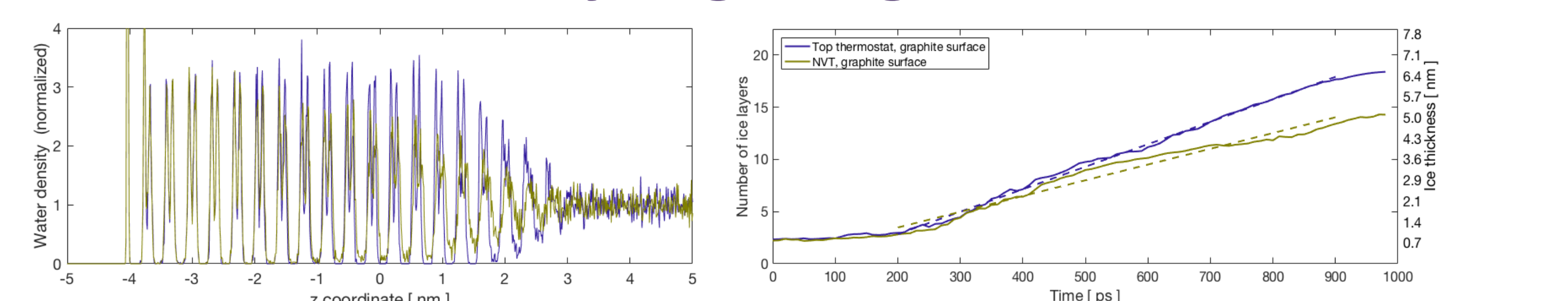


Perfect (001) surface with
bulk water at liquid density

(001) surface with step edge
along [100] with water film

(001) surface with double
layer pit with water film

Latent heat: analysing the growth rate of ice



Fractional ice layers: $n = (0.3 - \langle \rho \rangle) / 0.3$ at density (ρ) minima [Fraux, Doye JCP 2014]
Ice growth rate from lsq. fit: NVT: 5.39 nm/ns, top thermostat
(better treatment of latent heat from crystallization): 7.69 nm/ns.

OUTCOME

Successful implementation of the aerosol-droplet-ice particle interactions in a cloud resolving model

Validation of molecular ice nucleation models using direct comparison with experiments on chemically identical systems

Parameterization of ice nucleation for improved large scale cloud and climate models

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