Formation of 2D Ice Confined by Hydrophobic Nanopore

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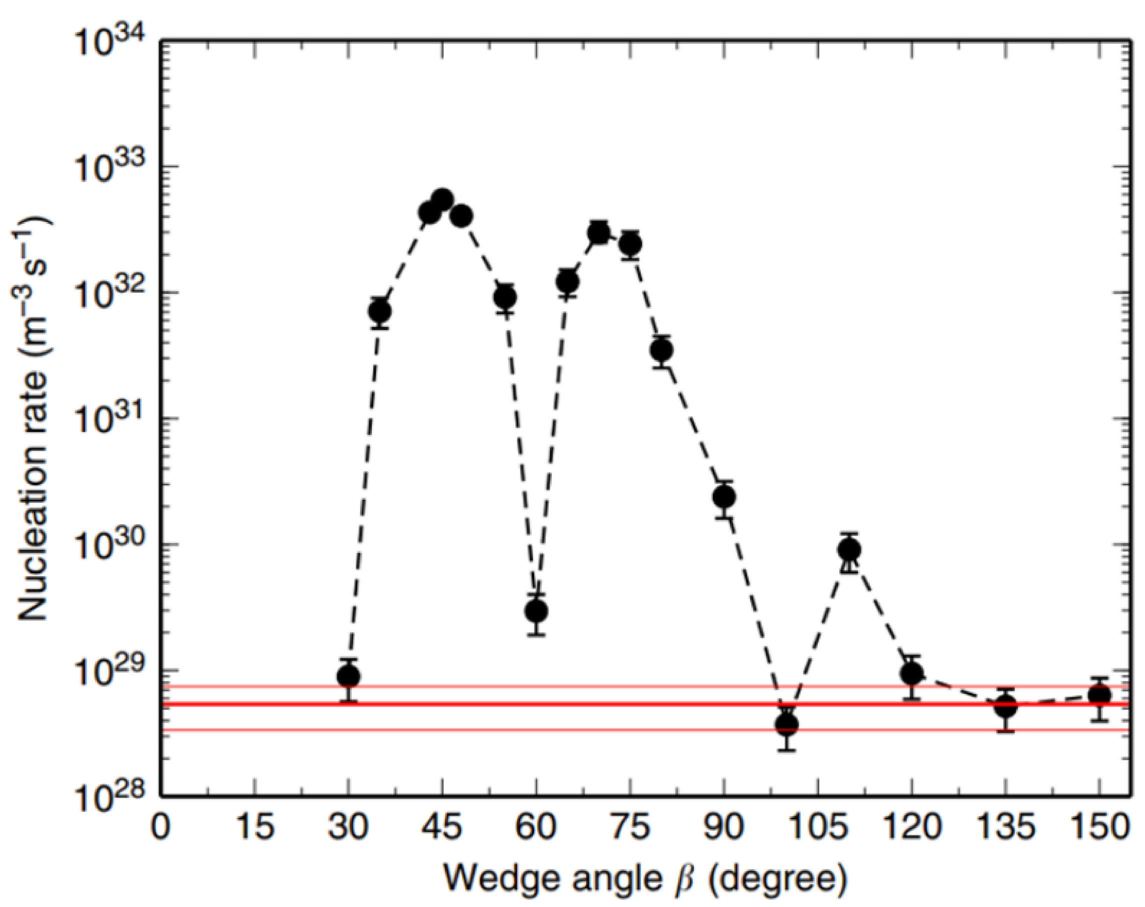
Background

- Clouds' lifetime and radiative properties are significantly affected by the freezing of water.
- Freezing is typically triggered by impurities in cloud droplets, such as mineral dust and bacteria.
- Extensive studies on ice nucleation of perfectly flat surface have been carried out. However, non-perfect geometries of impurities is poorly understood.

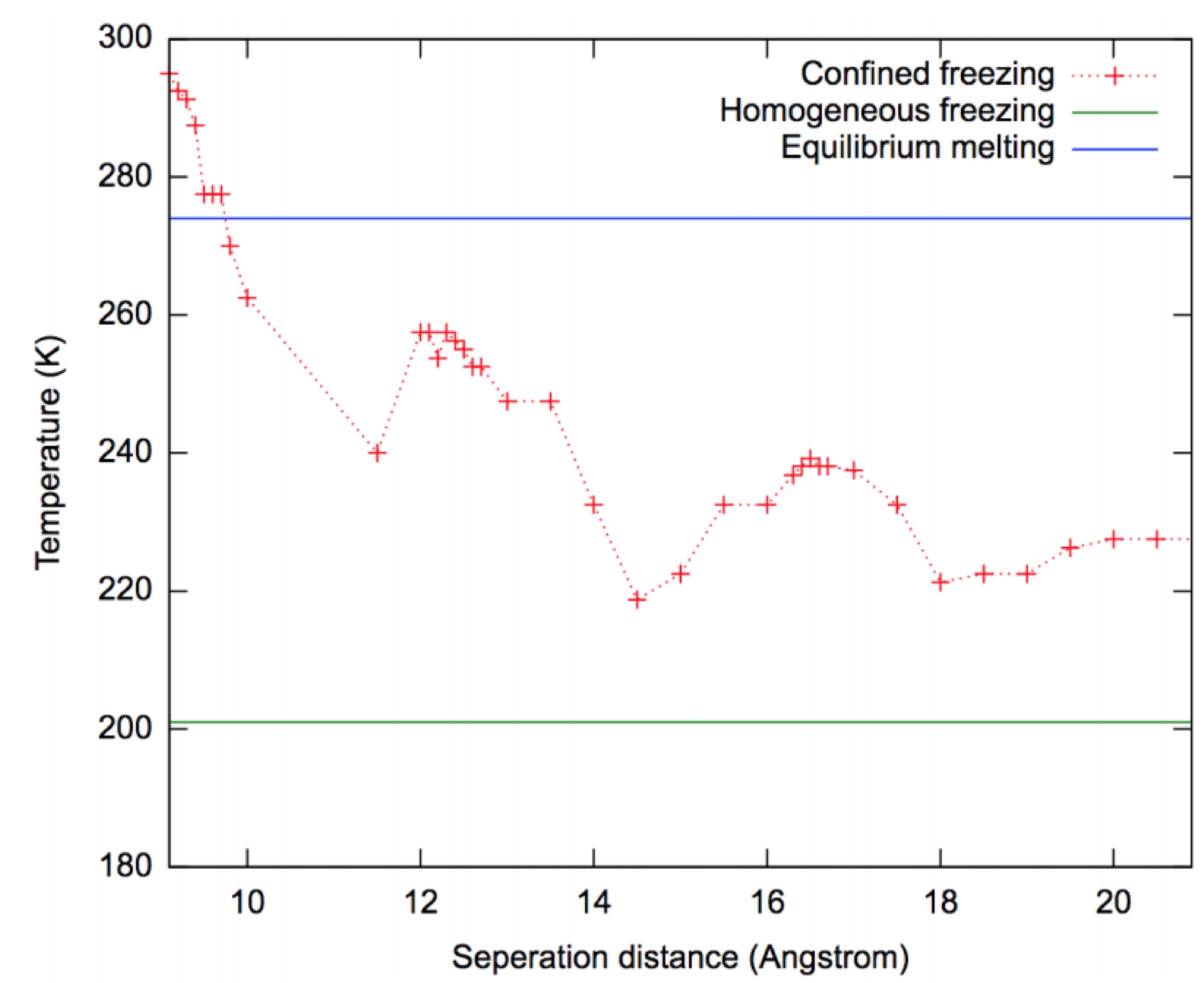


Calculated ice nucleation rate (black) within atomically sharp wedge at 230K. Red line indicates the calculated ice nucleation rate and it's uncertainty on a flat surface.

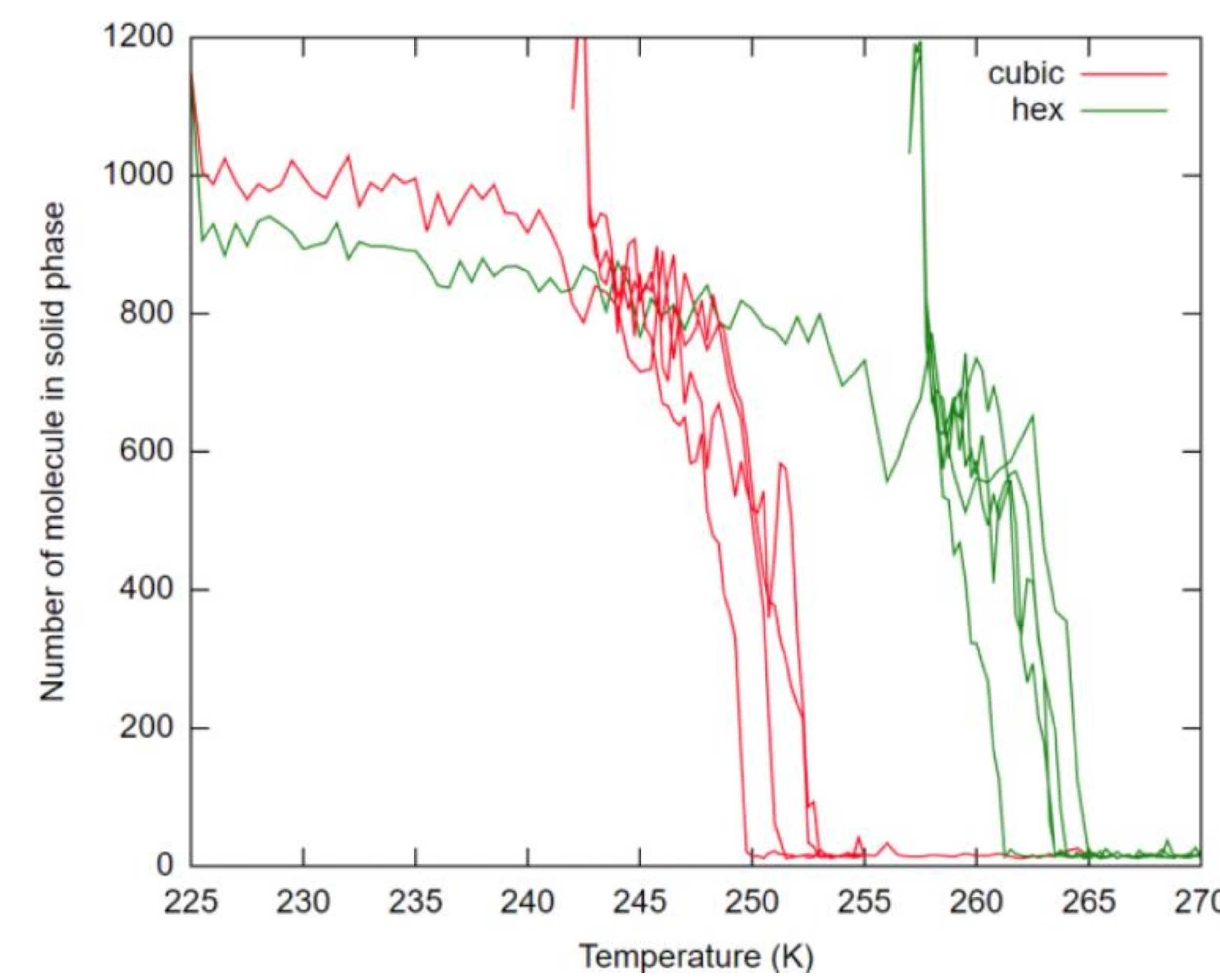
Methods

- Less resource-consuming coarse-grained mono-atomic water (mW) model.
- Graphene layers are used to create hydrophobic confinements.
- The interaction between carbon atom and water molecule is described by the two-body term of mW water model.
- Molecular dynamics simulations are carried out with LAMMPS.

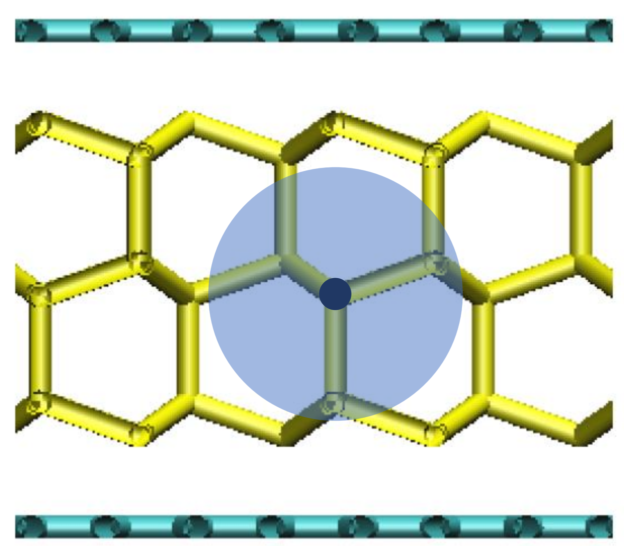
Results & Discussions



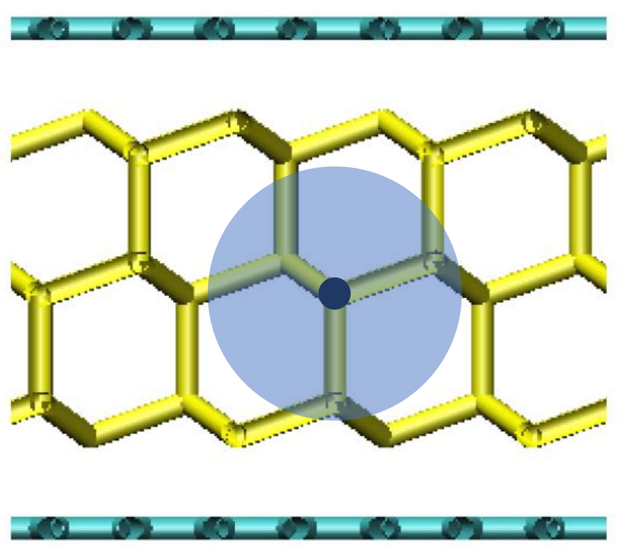
- The freezing temperature of confined ice exhibits a strong, non-monotonic dependence on the distance between graphene layers.
- The peak distances match the integer times of interlayer distance of ice plane.



- The melting of 3-layer hexagonal ice is 12K higher than 3-layer cubic ice.
- This large difference in melting temperature is in contrast to that in bulk ice, where there is only a 3K melting temperature difference between cubic and hexagonal.
- The absence of stacking disorder in trilayer ice originates from the higher thermodynamic stability of confined hexagonal 3-layer ice, rather than being a kinetic effect

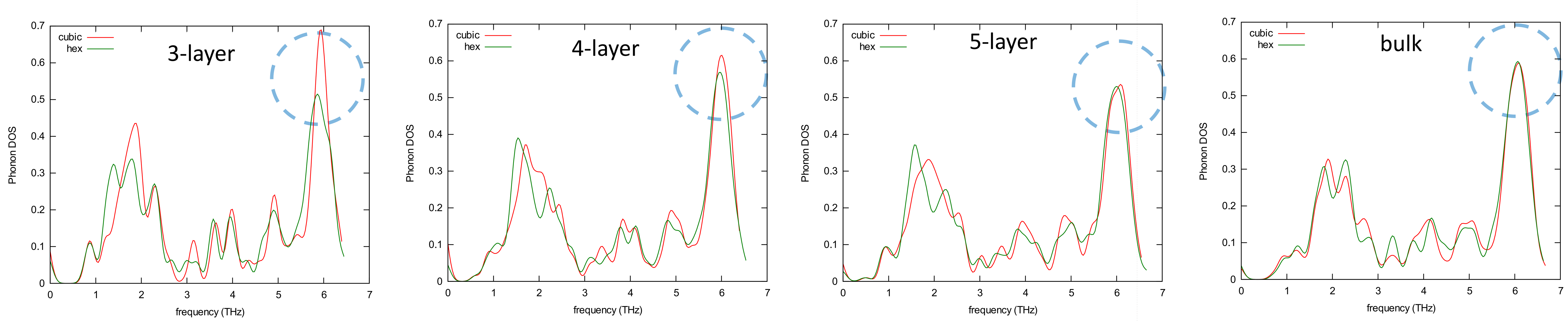


Hexagonal Ice



Cubic ice

- Hexagonal ice and cubic ice have the same potential energy.
- Each individual molecule can not distinguish two structures.



- Phonon density of state reveals the reason why hexagonal ice is more stable than cubic ice.
- 3-layer ice is 2D material.
- 5-layer ice could be considered as bulk ice.