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# Deep learning for unravelling features of heterogeneous ice nucleation

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Davies et al. (1) presented work aimed at predicting the ice-nucleating ability of several interfaces by means of a ready-to-use deep learning tool.

## Ice Nucleation in Nature Happens Heterogeneously

Water freezes in a wide variety of low-temperature natural environments, ranging from atmospheric clouds to soil and biological cells. When supercooled below the melting temperature, crystallites start homogeneously nucleating until liquid water completely transforms into ice (2, 3). The transition of liquid water into ice is relevant to atmospheric science, geology, and microbiology. Ice crystallization is also relevant to ecology, where ice-nucleating bacteria can damage plants via frosting, or to material science, where novel materials for controlled interfacial freezing can be designed.

Ice nucleation in nature cannot occur from mildly supercooled bulk water. When liquid water is supercooled down to 20° below melting, the ice nucleation rate is slower than the rate corresponding to one ice nucleus appearing in all water in the hydrosphere during the age of the universe (4). For this reason, ice nucleation has to happen heterogeneously, induced by the presence of interfaces of solid impurities operating as nucleating agents.

Heterogeneous nucleation of ice on aerosols of various origins is the main mechanism of ice formation in the atmosphere (5). This leads to the development of ice-rich clouds, which play an important role in mediating the amount of solar radiation reaching the Earth. Atomically flat carbon surfaces have been shown to promote heterogeneous ice nucleation, inducing layering in the nearby interfacial water (6).

Cold-adapted organisms are capable of producing antifreeze/ice-nucleating proteins to prevent/promote ice formation at temperatures below melting (7).

In the surroundings of *Pseudomonas syringae* bacteria, ice nucleation is enhanced by ad hoc ice-active sites with unique hydrophilic–hydrophobic patterns. Not only is ice nucleation efficiency promoted by the presence of ice-like or anchored clathrate motifs (8), but also, the hydrogen bonding at the water–bacteria contact imposes a structural ordering on the adjacent water network.

## Which Structural Features Should Characterize an Interface for It to be Considered a Good Ice Former?

Even though experimental or numerical studies on several materials have so far led to a deeper understanding of the mechanism behind heterogeneous ice nucleation (9), predicting the ice-nucleating abilities of a substrate based on its properties still remains an unattainable goal.

We are probably living in the golden age of machine learning (10), deeply connected with condensed matter physics, where an important goal is unraveling atomistic insights of many-body systems (11). To overcome timescale limitations of ab initio techniques and accuracy issues with force field methods (12), machine learning tools have been developed to provide accurate model potentials (13) for complex aqueous systems (14) ranging from water under nanoconfinement to water in contact with different surfaces.

To design materials capable of controlling ice formation, predicting ice-nucleating abilities of several substrates would be desirable. Recently, machine learning techniques have been tailored for a quantitative understanding of heterogeneous ice nucleation on several substrates (15). Intrinsic surface properties (i.e., the match between the surface's lattice to the low-index face of ice and the adsorption energy) together with features of interfacial water (i.e., a local ordering induced by the surface and a density decrease) were shown to play a key role in the ice-nucleating ability of a substrate.

To date, it remained unclear how to a priori predict the ice nucleation ability of a given material, and expensive computer simulations or experiments were needed to unravel the efficacy of an ice-nucleating agent.

## Machine Learning for Predicting Ice Nucleation Abilities of Surfaces

Davies et al. (1) have tackled this issue by developing a ready-to-use deep learning tool: "IcePic."

Making use of an in silico image of room temperature water in contact with several substrates, IcePic allows us to infer the nucleation ability far better than human predictions.

Interestingly, the numerical tool confirmed the relevance of the structure of contact water in affecting the nucleation properties, as predicted by experiments (16) and costly simulations (17, 18), and it provides physical insights on interfacial water.

This tool opens up avenues for investigating ice nucleation, with relevance in atmospheric science, geology, and microbiology.

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