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Computational Investigation of Surface Freezing in a Molecular Model of Water AMIR HAJI-AKBARI, Department of Chemical and Environmental Engineering, Yale University, PABLO DEBENEDETTI, Department of Chemical and Biological Engineering, Princeton University — Ice formation plays a pivotal role in atmospheric processes. Yet, its microscopic mechanism is difficult to determine from experiments. One of the biggest unresolved questions about ice formation in the atmosphere is whether a vapor-liquid interface enhances or suppresses freezing at its vicinity, a conundrum regarded as of the ten biggest unresolved questions about ice and snow [1]. Despite earlier suggestion that ice formation must be enhanced at a free interface [2], the experimental evidence for and against it are inconclusive. In this work, we address this question computationally and use a path sampling technique known as forward flux sampling to study the kinetics and mechanism of ice nucleation in freestanding nanofilms of supercooled water modeled using the TIP4P/Ice force field, one of the best molecular models of water. We observe that nucleation is almost seven orders of magnitude faster than the bulk in the film geometry. Yet, the nucleation process is homogeneous in nature, and starts not at the free surface, but within an interior region of the film that favors the formation of double diamond cages, and therefore the cubic polymorph of ice. [1] Bartels-Rauch, Nature, 494, 27 (2013). [2] Tabazadeh, *et al*, PNAS, 99, 15873 (2002).

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