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Exploring the coupling between surface crystallinity and surface hydrophilicity in heterogeneous ice nucleation YUANFEI BI, RAFFAELA CABRIOLU, TIANSHU LI, the Georege Washington University — Heterogeneous ice nucleation has significant influence in a variety of fields ranging from global climate change to intracellular freezing. Although its prevalence can be explained quantitatively by the classical nucleation theory [1], there is a lack of molecular level understanding of the key factors governing ice nucleation at the interface between water and ice nucleator. Here, by employing advanced molecular simulation, we show [2] that heterogeneous ice nucleation on graphitic surface is controlled by the coupling of surface crystallinity and surface hydrophilicity. Molecular level analysis shows that the crystalline graphitic surface with an appropriate hydrophilicity templates ice basal plane forming in the contact layer, thus significantly enhances its ice nucleation efficiency. Remarkably, the templating effect is found to transit from within the first contact layer of water to the second as the hydrophilicity increases, yielding an oscillating distinction between the crystalline and amorphous graphitic surfaces in their ice nucleation efficiencies. Our study sheds new light on the long-standing question of what constitutes a good ice nucleator. 1 R. Cabriolu and T. Li, Physical Review E 91, 052402 (2015). 2 Y. Bi, R. Cabriolu, and T. Li, arXiv:1510.01371 (2015).

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