Abstract Submitted
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A one-dimensional ice structure built from pentagons JAVIER CARRASCO, London Centre for Nanotechnology and Department of Chemistry, University College London; Fritz-Haber-Institut der Max-Planck-Gesellschaft, ANGELOS MICHAELIDES, London Centre for Nanotechnology and Department of Chemistry, University College London — Heterogeneous nucleation of water plays a key role in fields as diverse as atmospheric chemistry, astrophysics, and biology. Ice nucleation on metal surfaces offers an opportunity to watch this process unfold, providing a molecular-scale description at a well-defined, planar interface. We discuss a density-functional theory study on a metal surface specifically designed to understand such phenomena. Together with our colleges at the University of Liverpool, we found that the nanometer wide water-ice chains experimentally observed to nucleate and grow on Cu(110) are built from a face sharing arrangement of water pentagons [1]. The novel one-dimensional pentagon structure maximizes the water-metal bonding whilst simultaneously maintaining a strong hydrogen bonding network. These results reveal an unanticipated structural adaptability of water-ice films, demonstrating that the presence of the substrate can be sufficient to favor non-conventional structural units.

[1] J. Carrasco *et al.*, Nature Mater. **8**, 427 (2009).

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