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Enhanced configurational entropy in high-density nanoconfined bilayer ice FABIANO CORSETTI, Department of Materials and the Thomas Young Centre for Theory and Simulation of Materials, Imperial College London, London SW7 2AZ, United Kingdom, JON ZUBELTZU, EMILIO ARTACHO, CIC nanoGUNE, 20018 Donostia-San Sebastin, Spain — Understanding the structural tendencies of nanoconfined water is of great interest for nanoscience and biology, where nano/micro-sized objects may be separated by very few layers of water. We present a study of water confined to a 2D geometry by a featureless, chemically neutral potential, in order to characterize its intrinsic behaviour. We use molecular dynamics simulations with the TIP4P/2005 potential, combined with density-functional theory calculations with a non-local van der Waals density functional and an *ab initio* random structure search procedure. We propose a novel kind of crystal order in high-density nanoconfined bilayer ice. A first-order transition is observed between a low-temperature proton-ordered solid and a high-temperature proton-disordered solid. The latter is shown to possess crystalline order for the oxygen positions, arranged on a close-packed triangular lattice with AA stacking. Uniquely amongst the ice phases, the triangular bilayer is characterized by two levels of disorder (for the bonding network and for the protons) which results in a configurational entropy twice that of bulk ice.

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