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2D ice from first principles: structures and phase transitions JI CHEN, Thomas Young Centre, University College London, London Centre for nanotechnology, GEORG SCHUSTERITSCH, CHRIS J. PICKARD, Thomas Young Centre, University College London, University of Cambridge, CHRISTOPH G. SALZMANN, University College London, ANGELOS MICHAELIDES, Thomas Young Centre, University College London, London Centre for nanotechnology — Despite relevance to disparate areas such as cloud microphysics and tribology, major gaps in the understanding of the structures and phase transitions of low-dimensional water ice remain. Here we report a first principles study of confined 2D ice as a function of pressure. We find that at ambient pressure hexagonal and pentagonal monolayer structures are the two lowest enthalpy phases identified. Upon mild compression the pentagonal structure becomes the most stable and persists up to ca. 2 GPa at which point square and rhombic phases are stable. The square phase agrees with recent experimental observations of square ice confined within graphene sheets. We also find a double layer AA stacked square ice phase, which clarifies the difference between experimental observations and earlier force field simulations. This work provides a fresh perspective on 2D confined ice, highlighting the sensitivity of the structures observed to both the confining pressure and width.

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