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A Computational Study of the Growth of Hexagonal Ice. MAXWELL FULFORD, King's College London, UK, MATTEO SALVALAGLIO, UCL, UK, MICHELE PARRINELLO, ETH Zurich; USI Lugano, CARLA MOLTENI, King's College London, UK — Hexagonal ice (Ih) has two distinct crystallographic surfaces; a basal and prism surface. At low vapour pressures, Ih forms thin plates and elongated prisms, depending on the temperature. The macroscopic shape depends on the relative rate of growth of the basal and prism surfaces. The aim of our research is to estimate the relative rate of growth of the two surfaces for a range of temperatures and ultimately predict the shape of Ih, using computer simulations. Our simulations show the well-know phenomenon that the surface of ice lowers its interfacial free energy by forming a stable quasi-liquid layer (QLL). The QLL mediates crystal growth and has a thickness which varies with temperature and crystallographic surface. We use a combination of Molecular Dynamics and Metadynamics to study how the interfacial structure at the ice/quasi-liquid and quasi-liquid/vapour interfaces influence the adsorption potential, surface transport properties and growth shape..

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