Abstract Submitted
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A model of the ideal molecular surface BRYAN HENSON, LAURA SMILOWITZ, Los Alamos National Laboratory — We utilize two manifestations of the phenomena of the quasiliquid phase on the surface of molecular crystals to formulate a universal thermodynamic theory describing the thickness of the layer as a function of the liquid phase activity. We use direct measurements of the liquid thickness as a function of temperature and measurements of the acceleration of thermal decomposition as a function of temperature approaching the melting point to illustrate the mechanism. We show that given the existence of a liquid phase below the melting point the ideal liquid activity is necessarily a fixed function of the free energies of sublimation and vaporization. We use this activity to create a reduced formula for the liquid thickness generally applicable to the molecular surface. We provide a prediction of the mechanism and kinetics of quasiliquid formation and show that the phase exists as a metastable kinetic steady state. We show that to first order the principle controlling feature of the system is the configurational entropy of the liquid/solid interface, rather than the specifics of the surface potential energy. This is analogous to other bulk colligative phenomena such as ideal gas and solution theories, and is thus an ideal, universal formulation of inherent, thermodynamically driven, surface disorder.

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