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Orientational Defects in Ice Ih: An Interpretation of Electrical Conductivity Measurements MAURICE DE KONING, ALEX ANTONELLI, Universidade Estadual de Campinas, ANTONIO J.R. DA SILVA, ADALBERTO FAZZIO, Universidade de Sao Paulo — While the isolated water molecule is one of the simplest in Nature, the condensed phases of H_2O reveal many complex features that still elude complete understanding. An example concerns the role of crystal defects in the peculiar electrical properties of proton-disordered hexagonal ice Ih. When an electric field is applied to an ice specimen, it becomes polarized by the thermally activated reorientation of the molecular dipoles through the motion of Bjerrum defects, which represent local disruptions of the hydrogen-bond network. While the conceptual picture of these Bjerrum defects is now well established, a quantitative understanding of their properties is still lacking, rendering a direct interpretation of experimental electrical conductivity data difficult. In this work we present a first-principles study of the structure and energetics of Bjerrum defects in ice Ih and compare the results to experimental electrical conductivity data. While the DFT result for the activation energy is in good agreement with experiment, we find that its two components have quite different values. Aside from providing new insight into the fundamental parameters of the microscopic electrical theory of ice, our results suggest the activity of traps in doped ice in the temperature regime typically assumed to be controlled by the free migration of L-type Bjerrum defects.

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