First-principles Study of Stacking Faults in Ice Ih

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Using plane-wave density-functional-theory calculations, we evaluate formation energies for three types of stacking faults in the proton disordered hexagonal structure of water, known as ice Ih. For each type of stacking fault we generate four different cells corresponding to different proton-disorder configurations and compute the associated stacking-fault energies. Given that ice is a molecular crystal, it is necessary to correct the hydrogen bounds between water molecules adjacent to the plane of the fault. Such corrections induce a nonzero dipole moment of the cell. In order to correct for the spurious energy contributions associated with the periodic array of dipoles we use the approach developed in [1]. The results indicate that the formation energy associated with the stacking faults is very small, in agreement with [2,3]. In the context of the mechanical properties of ice, this result implies a strong dissociation tendency of dislocations on the basal plane into partial dislocations. In addition to the intrinsic stacking-fault configurations, we determine the generalized stacking-fault energy surface of the faults. The results will be used in a Peierls-Nabarro-type approach to study the core structure and mobility of dislocations in the basal plane of ice Ih.

