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First-principles study of molecular point defects in ice Ih MAURICE DE KONING, ALEX ANTONELLI, Universidade Estadual de Campinas, ANTONIO J.R. DA SILVA, ADALBERTO FAZZIO, Universidade de Sao Paulo — We present a first-principles study of the structure and energetics of molecular point defects in ice Ih [1]. Our approach is based on a DFT-GGA description, utilizing a periodic supercell containing 96 water molecules. We compute the formation free energies and corresponding thermal equilibrium concentrations as a function of temperature for the molecular vacancy and 3 different interstitial structures: the Tc, Tu and Bc configurations. The latter involves bonding to the surrounding lattice, whereas the first two do not. The results indicate that, due to its bonding to the surrounding lattice, the equilibrium concentration of the Bc interstitial is larger than that of the Tc and Tu structures, suggesting that the Bc structure is the preferred interstitial configuration in ice Ih. Comparison with the molecular vacancy, on the other hand, indicates that the vacancy is expected to be the overall dominant molecular point defect in ice Ih, at least for temperatures below T $\approx$ 200 K. Due to the elevated formation entropy of the Bc interstitial, however, a crossover scenario in which the Bc interstitial becomes favored at temperatures below the melting point, as has been suggested experimentally, is conceivable.
[1] M. de Koning, A. Antonelli, A.J.R. da Silva and A. Fazzio, Phys. Rev. Lett. **97**, 155501 (2006).

Maurice de Koning
Universidade Estadual de Campinas

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