Effect of proton disorder in the excited state properties of ice

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Ordinary ice has a hexagonal crystal structure (ice Ih). A metastable cubic crystalline variant of ice exists, where oxygen atoms are arranged in a diamond structure (ice Ic), and the hydrogen ones are disordered, still obeying the Pauling ice rules. It is produced at temperatures between 130-150 K, and is stable for up to 200 K, when it transforms into ice Ih. The proton disorder in ice has a role in several properties such as growth condition and thermal properties [1,2] and many works about phase transitions from proton disordered to proton ordered ices can be found in literature. Moreover, depending on the proton ordering, some ice phases can also present ferroelectric or antiferroelectric behaviors [3,4].

In recent years, the excited state properties of hexagonal ice have been studied within many-body perturbation theory (MBPT) [5]. The electronic and optical properties of cubic ice, instead, have never been calculated accurately: only tight-binding [6,7] and density functional theory (DFT) [8,9] calculations have appeared in the literature. Moreover, in several of these studies the proton disorder is not taken into consideration. Here, we present MBPT calculations of the electronic and optical properties of cubic ice exploiting model cells with different level of proton disorder and we compare our results with ice Ih and with liquid water.

Preliminary results on ice surfaces are also discussed.

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