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Enhancement of dipolar dynamics and hydrogen ordering: Dielectric studies of doping effects

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The crystalline ices can be divided into two groups, the hydrogen disordered and the hydrogen ordered ices. Phase transitions between ordered/disordered pairs that share the same oxygen lattice require the rearrangement of hydrogen bonds. These reorientational processes can only take place if point defects are present that locally violate the Bernal-Fowler ice rules, and the concentration of such defects can be increased by the addition of dopants. A large variety of dopants has been examined so far and in principle acid, base, and salt dopants can be used. Their effectiveness in enhancing the charge dynamics and enabling the formation of ordered phases is still in the focus of intensive research [1].

Dielectric spectroscopy is a method well suited to examine the potential enhancement of dipolar dynamics. In the present contribution we study the high-pressure ice phases ice V, VI, and XII. In these phases the number of intrinsic point defects is too low to induce a hydrogen ordering to the less entropic partners XIII, XV, and XIV, respectively. However, the addition of dopants increases the dynamics of the dipolar relaxation and can promote the transition to their hydrogen ordered partners. We compare a variety of dopants (HCl, HBr, HF, KOH, NH3) and present an overview regarding the efficiency of these dopants in ice V, VI, and XII and in the resulting cubic and hexagonal ices that form upon heating [2,3].

We find HCl to be the dopant that enhances the dipolar dynamics the most and in agreement with previous work [4,5] we also observe order-disorder-transitions in the HCl doped ices V, VI, and XII. KOH, the dopant that is known to be the most effective in hexagonal ice, is one of the least effective in these high-pressure ices.

Furthermore, we investigate the enhancement of dynamics in ice XII as a function of the HCl-dopant concentration with the objective to determine the minimum amount of HCl needed to induce hydrogen ordering and to check whether there is a maximum of enhancement that cannot be exceeded even if large amounts of the dopant are added.

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[1] C. G. Salzmann, P. G. Radaelli, B. Slater, and J. L. Finney, Phys. Chem. Chem. Phys. 13, 18468 (2011)
[2] K. W. Köster, A. Raidt, V. Fuentes Landete, C. Gainaru, T. Loerting, and R. Böhmer, Phys. Rev. B, 94, 184306 (2016)
[3] K. W. Köster, V. Fuentes Landete, A. Raidt, M. Seidl, C. Gainaru, T. Loerting, and R. Böhmer, Nat. Commun. 6, 7349 (2015); K. W. Köster, V. Fuentes Landete, A. Raidt, M. Seidl, C. Gainaru, T. Loerting, and R. Böhmer, Erratum (submitted)
[4] C. G. Salzmann, P. G. Radaelli, A. Hallbrucker, E. Mayer, and J. L. Finney, Science 311, 5768 (2006)
[5] C. G. Salzmann, P. G. Radaelli, E. Mayer, and J. L. Finney, Phys. Rev. Lett. 103, 105701 (2009)

Significance statement

The dipolar dynamics in ice can be enhanced by adding dopants. In many ice phases dopants are needed to induce the phase transition from a hydrogen disordered to a hydrogen ordered phase. We study the dopant efficiency in several high-pressure ice phases and in cubic and hexagonal ice.

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