Structural effect induced by excess charges on ice systems

Francesca Baletto[1,2], Carlo Cavazzoni[3] and Sandro Scandolo[2]

[1] Department of Materials Science and Engineering, MIT, Cambridge, MA
[2] ICTP and INFM/Democritos, Trieste, Italy
[3] CINECA and INFM/S3, Bologna, Italy

The knowledge of the physical properties of ice surface and water clusters have important implications in atmospheric chemistry, electro-chemistry, and radiation physics; especially, identifying the existence of stable surface-bound states for excess electrons is one of the hot point in material science. By means of first-principles molecular dynamics, we find that excess electrons (EE) induce a structural reconstruction of the ice surface on a time scale of a fraction of a picosecond which stabilizes the EE in a surface-bound. Such mechanism explains the remarkable stability of large cluster isomers with EE in surface states, which provides a microscopical picture of the surface sites relevant for the heterogeneous chemistry on atmospheric ice [1].

[1] F.Baletto, C. Cavazzoni and S. Scandolo. Phys. Rev. Lett. 95, 176801 (2005).