The behaviour of water molecules at the surfaces of quartz and a SiO_2 nanorod

Zhimei Du & Nora de Leeuw

School of Crystallography,
Birkbeck College,
University of London,
Malet Street,
London WC1E, 7HX, UK.
e−mail: z.du@mail.cryst.bbk.ac.uk

Quartz is the most common mineral on the surface of the Earth, which exists in nearly every geological environment and is a component of almost every rock type. C onsiderable amounts of water can be incorporated in the quartz structure with profound effects on many physical properties, such as diffusion rates, crystal strength and melting point. The influence of water on quartz is thus an interesting subject and a wide range of investigations has been conducted in recent years to study the interaction of water with silica, via both experimental and theoretical work. However, few studies have been performed on the interaction of quartz surfaces with water.

We present preliminary work on the interaction of water with surface sites of α−quartz and a SiO_2 nano−rod, which is constructed of fully coordinated SiO_4 terahedral units. Computational studies of the behaviour of molecules with nano−structures are very important, as experimental studies of such phenomena are still difficult to perform. The SiO_2 nano−rod will be used as a benchmark to investigate the hydrolytic weakening of silicate nano−particles. Both *ab initio* and classical atomistic methods have been employed to calculate the stabilities and hydration energies of the adsorption of water at the α−quartz (0001) surface and the SiO_2 nanorod. Water is found to chemisorb dissociatively onto the quartz surface, as the low−coordinated surface Si and O species thus increase their coordination number to the bulk value of four and two respectively. However, at the nano−rod sites, dissociative adsorption is only energetically preferred over associative physisorption of water at the ends of the nano−rod where the Si and O atoms are in a more strained environment.