Ab initio modeling of silica-based materials

Piero Ugliengo – Dipartimento Chimica IFM – Via P. Giuria 7. 10125 Torino. ITALY
piero.ugliengo@unito.it

The surface of silica-based materials is covered of silanol groups which impart adsorbitive features dependent on their concentration and type. Because of their amorphous nature, few structural details are knwon from experiment, so that it is expected that ab-initio simulation will play an important role for the understanding of the microscopic details at the surface. In this talk new results from our own work will be presented about silica surfaces at different OH coverages either bare or in interaction with water. The computed B3LYP vibrational frequencies of the silica surfaces and the energy of interaction of water are in good agreement with the available experimental data. The discussion will also cover the "hydrogarnet defect" which is likely to be present in crystalline silica-based materials of microporous nature. The adopted approach is based on the periodic DFT ab-initio calculation using localized basis functions as implemented in the CRYSTAL03 computer code developed by the Theoretical Chemistry Group of the University of Torino.