Nanostructured Surfaces

Molecular dynamics of water adsorbed on the surface of mesoporous silica material SBA-15

A. Kiwilsza[1,2]

[1] *Faculty of Physics, Adam Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland.*
E-mail: annamk@amu.edu.pl

[2] *NanoBioMedical Center, Adam Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland.*

Mesoporous silica materials with characteristic hexagonally arranged structure of pores (SBA-15, MCM-41) are nowadays a subject of great interest. Due to their unique properties (excellent sorptivity, well-defined pore size, thermal and mechanical stability as well as high biocompatibility and low toxicity), they have been implemented in e.g. chemical catalysis, environmental purification or biomedicine.

As it was shown in literature, while considering them in such applications, even after drying procedures, water adsorbed on their walls cannot be omitted. Especially, if the amount of it is quite low (comparable to one or two monolayers), some unusual surface effects are probable to be observed.

In this study molecular dynamics of water molecules adsorbed on the silica surface of SBA-15 material (surface area 710 m^2/g, pore size 5.55 nm) with 6.1% of water content (15% of pore filling) were investigated using mostly NMR and QENS techniques. As a result of the strong interaction with silica surface, translational diffusion in the system was excluded, but two types of stochastic localised motions were identified and both described using a model of 2-site jump. For both motions the characteristic jump distances, correlation times as well as activation energies have been extracted and found to differ significantly. On this basis, the faster motion was ascribed to jumps of water molecules between neighbouring positions (d = 2.5 Å, = 3 ps at 300 K, and $E_a = 5.2 \pm 0.2$ kJ/mol from NMR data and 5.6 ± 1.1 kJ/mol from QENS), while the slower one (with temperature dependent distance) was ascribed to jumps of water molecules between more spatially separated positions (d = 2.9 – 4.3 Å, = 20 ps at 300 K, and $E_a = 16.1 \pm 0.3$ kJ/mol from NMR and 17.3 ± 0.3 kJ/mol from QENS data). The presence of another fast motion (= 4 ps at 150 K) was also suggested, but its geometry was impossible to be determined experimentally.