Role of the Substrate Surface Morphology and Physicochemical Properties for Molecular Transport in the Vicinal Water: Aspect of Continuity of Dynamic Hydrogen Bond Network

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Extended Abstract

Water is omnipresent and indispensable for life as we know it. Human kind exploited the solvent power of liquid water and built around it, more and more consciously and knowingly with time, majority of our bio - and chemical activities. Today, we are deeply aware of the important role of hydrogen bond (H-bond) networking between adjacent waters in the solvent power of water. Nonetheless, we do not really understand how it works. Consequently, a lot of effort has been devoted to evidence experimentally and model the network and its dynamics. Present state of understanding is that in the bulk liquid water H-bond network is a rapidly fluctuating structure, with each water participating in twice as many H bonds per molecule as in the isolated state [1].

We extended the percolation studies onto the silica surface for its - already mentioned - topological and chemical alikeness to the biological ones. On the just wet surface of fumed silica Aerosil grains we found that the percolation transition occurs when amount of water corresponds to the state of a residual film, so charge transport is also two-dimensional in nature. But, intriguingly, it shows up on dehydration much earlier, i.e., when the average aqueous layer is no more than triple monolayer thick [2-5].

The essence of the method rests in simultaneous observation of sample conductivity changes and the rate of water loss from the sample as a function of time. These studies will, in parallel, provide the key information on the electrical conductivity during the free drying to the environment, especially determination of the conductivity percolation threshold the residual surface layer of water at the silica. Percolation threshold plays, in the dehydration kinetics study, a role of a "label" that allows identification of the moment when there is no more than 2-3 monolayers thick layer of water at the surface of studied sample. At the same time, percolation parameters, the threshold and the critical exponent, are also a measure of the nature of the continuum of hydrogen bonds in the final layer of water: a mesh vs. a conductive film.

We would like to present results on conductivity percolation different porous materials and zeolites such as SBA-15, MCM-41, ZSM-5 with a different Si/Al ratio. The results show additionally that possible is to determine properly the surface of the sample by research carried out in varying degrees of start hydration. The materials were tested with different levels of hydration. Exemplary results for MCM-41 are shown in Figure 1. On the Figure 2 can be observed relation between S from a, where a is the slope, and S is surface area of the sample determined by BET method. Chart has a high degree of linearity. Moreover, the equation of the matched line allows to estimate surface area of a sample based on the slope of h^* to h_0. Surface area values calculated by this method are compatible, within a range of error, values obtained using nitrogen sorption.
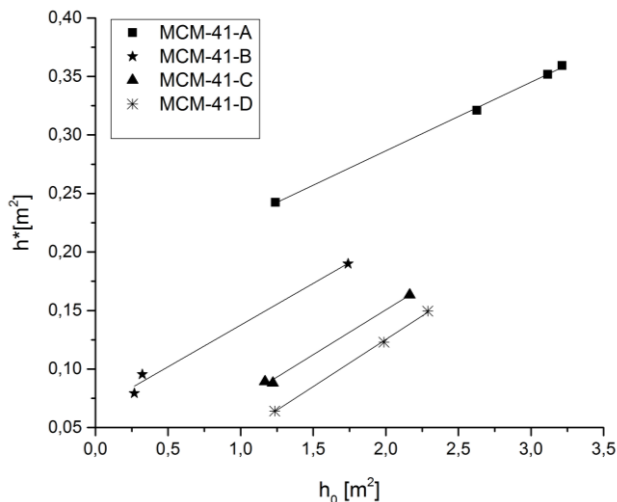
Fig. 1: Relation between initial hydration level h0 and hydration level in percolation threshold h*, obtained for studied MCM-41 samples. Each line represents linear regression result for samples from the same synthesis.
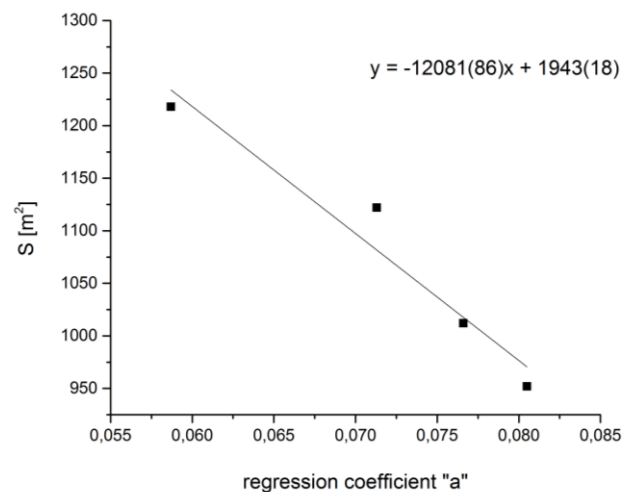

Fig. 2: Relationship between slope regression coefficient "a" and surface area for each sample with are presented together with the linear regression line and prospective results.

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