## КОЛОКВИУМ "АЛЕКСЕЙ ШЕЛУДКО" СЕКЦИЯ "ПОВЪРХНОСТИ И КОЛОИДИ" ИНСТИТУТ ПО ФИЗИКОХИМИЯ НА БАН

## СЪОБЩЕНИЕ

На 10 февруари 2017 г. (петък) от 11:00 часа в зала "Болцман" на ИФХ-БАН, ще се проведе заседание на Колоквиума със следния дневен ред:

1. Доклад на Веселин Тончев на тема:

## "THE FRACTAL DIMENSION OF ICE ON THE NANOSCALE: NUMERICAL PERSPECTIVE"

We provide a numerical perspective on the dependence of fractal dimension of ice clusters on temperature reported recently [S.-C. Heidorn et al., Chem. Phys. Lett. 665, (2016) 1–5]. In our model an initial population of particles is placed on a square lattice with an initial seed (nucleus) in the center. The sticking of diffusing particle to the growing cluster occurs according to a Cellular Automaton rule - when a nearest neighbor to even one particle from the cluster. This rule is executed in parallel for all such particles. In a complementary module, called diffusional update, all nonaggregated particles try sequentially a diffusional hop. Increasing the number nDS of such updates per growth one causes transition from diffusion-limited (nDS=1) to kinetics-limited (nDS>>1) growth mode. It is quantified by an increase of the cluster's fractal dimension Df. We obtain the dependence of Df on nDS and attribute the seeming deviations from the experimental data in the region of higher temperatures/high nDS values to the increase of the attachment rate. Additionally, we monitor properties that are hard to be assessed in experiments, such as the timeevolution of the crystallization rate and the ratio of aggregated particles in different coordination.

2. Разни (съобщения, организационни и др. въпроси).