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6th International Conference on

Physical and Theoretical Chemistry

September 02-03, 2019 | Zurich, Switzerland

Thermodynamics of 2D liquids, crystals and orientational ordering in molecular layers on solid surfaces: Kinetic monte carlo simulation

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There is a significant progress in the part of physical chemistry dealing with thin films, adsorption, coating and other surface phenomena. Sophisticated methods have been developed for the design networks of organic molecules, visualization and description of the structure of molecular layers. However, not much is known on thermodynamics of two-dimensional crystalline phases. The aim of this study is to show how the chemical potential of the crystalline molecular layer can be determined. We developed a methodology based on a kinetic Monte Carlo simulation of the gas-solid system in the cell with a variable external potential imposed on the gas phase. At equilibrium the chemical potential is the same over the cell and, therefore, this technique guaranties its reliable determination in the solid phase as that in the gas phase is easily evaluated. This approach proved to be very efficient in studying thermodynamic properties of contact layers of argon, krypton, nitrogen and hydrogen on solid surfaces and confined in nanoporous materials at cryogenic temperatures, as well as the melting and orientational (N2) long-to-short order transitions. The most challenging task is thermodynamic behavior of orientationally ordered layers formed by relatively large organic molecules. The reason is an extremely small primary molecular flux from the crystal and, therefore, its negligible contribution to the chemical potential compared to the secondary (reflected) flux. Nonetheless, the presence of the gas-solid interface allows us to circumvent the problem. Thus, we have successfully modeled the structures formed by trimesic acid and determined thermodynamic potentials and entropy of the chicken-wire structure and several flower-like polymorphs. From our viewpoint, the method has a significant potential for analysis of 2D crystals, their growth, thermodynamic stability, orientational and first order transitions.

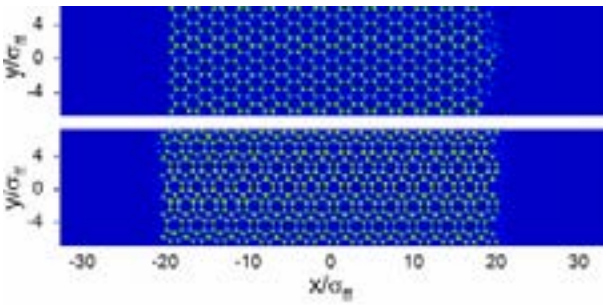

Figure 1: 2D gas-solid system for the chicken-wire (upper panel) and flower-like (bottom panel) structures of trimesic acid. Modeling with the kinetic Monte Carlo.

Recent Publications

1. Ustinov EA (2019) Kinetic Monte Carlo approach for molecular modeling of adsorption. Current Opinion in Chemical Engineering 24: 1-11.
2. Akimenko SS, Gorbunov VA, Ustinov EA (2019) Heat capacity and heat of adsorption at orientational phase transition in nitrogen monolayer on graphite. Adsorption 25: 555-565.

3. Ustinov EA (2018) Fluid–solid phase transition in molecular layers adsorbed on a smooth surface: A new insight from molecular simulations. J Phys Chem C 122: 23591-23599.
4. Ustinov EA, Gorbunov VA, Akimenko SS (2018) From simulation to thermodynamics of orientational transitions in molecular layers: Nitrogen contact layer on solids. J Phys Chem C 122: 2897-2908.
5. Ustinov EA (2017) Efficient chemical potential evaluation with kinetic Monte Carlo method and non-uniform external potential: Lennard-Jones fluid, liquid, and solid. J Chem Phys 147: 014105.
6. Bartels L (2010) Tailoring molecular layers at metal surfaces. Nature chemistry 2: 87-95.

Biography

Eugene Ustinov, Doctor in Physical Chemistry, Professor, is now a Leading Researcher at Ioffe Institute of Russian Academy of Sciences (Saint Petersburg, Russian Federation). He received his Doctor degree (1990) from the Institute of Physical Chemistry, Russian Academy of Sciences. His research interests focus on molecular modeling of the gas adsorption on surfaces and in confined volume of nanoporous materials at cryogenic temperatures; phase coexistence; two-dimensional first-order phase transition and orientational transition in molecular layers on solid surfaces. Eugene Ustinov has proposed a methodology for determination of the chemical potential and other thermodynamic functions of crystalline molecular layers using molecular simulation with a renewed version of the kinetic Monte Carlo method. He worked several times at the University of Queensland, Australia as a Visiting Professor. Eugene Ustinov has published more than 140 papers in peer-reviewed journals.

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