Novel approaches to computer simulation of self-assembled monolayers

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Discovery of novel self-assembled surface structures and it's applications, analysis of their stability and optimal growth conditions greatly benefit from computational studies of their atomistic models with statistical physics methods. Phase diagrams, adsorption isotherms, critical temperatures are routinely provided by computational experiments. But further development of surface self-assembly techniques pose new challenges to computation and simulation methods. Complex phase diagrams with numerous phases, narrow areas of existence and close phase transition points are hard to analyze with classical Monte Carlo methods. The vicinity of phase transitions causes critical slowing down phenomena, so it is very hard to get representative sample or at least some robust convergence criteria.

We think that another approaches are worth attention today. Tensor networks abstraction is a novel language of linear algebra that is natural for description of lattice physical systems, both quantum and classical ones [1]. Given a tensor network model of the adsorption system one can efficiently apply both transfer-matrix method and real-space renormalization approach. Transfer-matrix method gives numerically exact results with clear accuracy and work well near phase transitions that is crucial for systems with cascade of phases [2]. Renormalization approach obviate finite-size effects that always cast doubts upon results of computer simulations, especially for systems with large unit cells phases. Tensor network formulation of a computational task enables one to use recent advances in optimization of tensor network contraction algorithms as well as robust libraries of linear algebra subroutines. Given description of adsorption complexes and lateral interactions between them it is possible to build a tensor network model for any adsorption system. But in case of large complex molecules and numerous adsorbing molecules or adsorption complexes, building of a tensor network model is a tedious and error prone task. We propose the computer code SuSMoST (Surface Science Modelling and Simulation Toolkit [3]) to be used for automation of tensor network modeling of adsorption systems. Taking geometry and lateral interaction energies of adsorption complexes SuSMoST generates tensor network model that can be studied with SuSMoST modules or with any other tools.

References:
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