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Surface Science Modelling and Simulation Toolkit - bridging the gap between theory and experiment for self-assembled monolayers

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Recent advances in experimental techniques revealed a huge variety of structures that emerge in adsorption monolayers. For their practical application it is necessary to develop methods and tools of rational design of self-assembly processes. Drug industry experience proves that for rational design of molecular systems, computer modeling tools are invaluable. Using computer models the most promising molecules and parameter ranges can be chosen for experimental checks. Surface science routinely use methods of density functional theory (DFT) and molecular dynamics, largely due to existence of robust computer codes that allow "black box"usage. But outcomes of these methods are hard to compare with experiments. Statistical physics methods predict equilibrium properties and are much closer to experimental capabilities. In many studies such methods (Monte Carlo generally) implemented in in-house codes are used for investigation of specific systems. But exploratory researches need a universal yet efficient code. We have generalized our experience in computational studies of self-assembled monolayers in Surface Science Modeling and Simulation Toolkit (SuSMoST) and offer it to surface science community –http://susmost.com/ (supported by Russian Scientific Fund, project No 17-71-20053). The SuSMoST code is based on the general lattice model [1] that is able to describe a wide range of adsorption systems. Being formulated on tensor-network language it provides a common ground for several efficient algorithms with various accuracy and costs (Monte Carlo, transfer-matrix, renormalization approach). SuSMoST automates many tasks of theoretical analysis of adsorption systems: computation of lateral interaction energies with DFT, phase diagram estimation, calculation of phase transition points, isotherms and isobars plotting.

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[1] S.S. Akimenko, V.A. Gorbunov, A.V. Myshlyavtsev, P V. Stishenko, Physical Review E 93 (2016) 062804.

Primary author: STISHENKO, Pavel (Omsk State Technical University)

Co-authors: Mrs ANISIMOVA, Galina (Omsk State Technical University); GORBUNOV, Vitaly (Omsk state technical university); Mrs FADEEVA, Anastasia (Omsk State Technical University); FEFELOV, Vasilily (Omsk state technical university); Prof. MYSHLYAVTSEV, Alexander (Omsk State Technical University); Prof. MYSHLYAVTSEVA, Marta (Omsk State Technical University); Dr AKIMENKO, Sergey (Omsk State Technical University)

Presenter: STISHENKO, Pavel (Omsk State Technical University)

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