A unified lattice model and modern statistical methods implemented in Surface Science Modeling and Simulation Toolkit

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Self-assembly of molecular monolayers on solid surfaces has a great potential for mass production of nanodevices and new materials. The development of experimental techniques, such as atomic-resolution microscopy, made it possible to see a huge amount of ordered structures formed by adsorbed molecules. Nowadays, the attention of researchers is focused on the development of processes for controllable self-assembly of nanostructures with desired properties [1,2]. It requires special theoretical tools that allow to predict *in silico* the self-assembly and properties of the monolayers. The time scale of self-assembly processes often significantly exceeds the typical time integration step in classical molecular dynamics. Thus, it is very difficult to obtain a representative sample even with the advanced sampling techniques.

To simulate complex adsorption systems, we propose the Surface Science Modeling and Simulation Toolkit (SuSMoST). It includes a number of utilities and implementations of statistical physics algorithms that allow to predict or explain the structure and thermodynamic properties of adsorbed monolayers. SuSMOST automatically builds formal graph and tensor-network models from atomic description of adsorption complexes. It aids *ab initio* calculations of interactions between adsorbed species. With methods of various nature SuSMoST generates representative samples of adsorption layers and computes its thermodynamic quantities such as free energy, adsorption layer coverage and density, heat capacity, entropy.

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References

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2. Levchenko I. et al., *Advanced Materials* **30** (2018), 1702226.