TENSOR NETWORK APPROACH FOR MODELING THERMODYNAMIC PROPERTIES OF ADSORPTION SYSTEMS WITH MANY-BODY INTERACTIONS

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Thermodynamic properties of adsorption monolayers are determined by the nature of intermolecular interactions. Most theoretical studies are restricted to pairwise intermolecular potentials. The reason is the computational complexity of models with many-body interactions.

On the other side, quantum chemical calculations show the substantial contribution of many-body interactions in some cases [1]. These interactions can even lead to qualitative changes in the system behavior [2].

We have developed a unified tensor (UT) algorithm for lattice gas models of adsorption layers. This algorithm efficiently incorporates many-body interactions up to the third nearest neighbor in adsorption monolayers. In contrast to classical methods (Monte Carlo, transfer matrix), where accounting for such interactions is challenging, the tensor network approach affects only the tensor network construction stage. This opens up possibilities for the thermodynamic analysis of complex quasi-2D systems.

The UT algorithm was applied to the model metal-organic layer of 1,3,5-tris(4-pyridyl)benzene (TPyB) and copper on the Au(111) surface. This system is of interest for the fabrication of metal-organic nanostructures. The interaction energies were calculated using density functional theory. It was shown that these energies cannot be reduced to combinations of pairwise interactions.

Adsorption isotherm calculations revealed both quantitative and qualitative differences in the phase behavior of the system when many-body interactions were taken into account. The stability regions of ordered phases shift along the chemical potential (or gas phase pressure) axis. Qualitatively, several types of changes occur. Low-density phases disappear, while the thermal stability of dense ordered structures, such as the "superflower" phase, can be significantly reduced. Many-body interactions lead to disordered configurations with increased layer density. It is driven by the filling of the surface with copper atoms.

The proposed approach demonstrates high efficiency in studying complex adsorption systems with many-body interactions. The developed algorithm can be used to predict the thermodynamic properties of new molecular and metal-organic monolayers, which are promising for catalysis, nanoelectronics, and sensing.

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