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Coordination self-assembly of terephthalic acid molecules and Fe on Cu(100) surface: phase diagram from statistical simulation

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Molecular self-assembly is the most promising approach for the direct preparation of functional nanomaterials. Recently, the coordination-driven self-assembly are increasingly being used to create metal-organic structures of varying complexity on the solid surface: discrete polygons, cages, one-dimensional polymers, two-dimensional porous networks [1,2]. In comparison with other non-covalent interactions, the metal-ligand coordination is superior. Despite the high binding energy, it is reversible and characterized by high directionality and selectivity. In addition, surface-confined metal-organic networks have greater thermal stability than other 2D supramolecular structures based, for example, on hydrogen bonds motifs.
In this contribution, we propose a detailed lattice gas model of contact monolayer of terephtalic acid molecules and Fe atoms on Cu(100) surface under ultra-high vacuum conditions, taking into account the surface mediation effects. The model was investigated with Monte Carlo methods and tensor-network approach as implemented in the SUSMOST code [3]. We have explored the effect of metal-ligand partial pressures ratio and temperature on the structure of adsorption layer. The simple lattice model allows us to determine not only the possible structures of the adlayer, but also the thermodynamic conditions of the phase existence in terms of partial pressures (chemical potentials in gas phase) of the components. Our results are in good agreement with the experimental data [4,5]. The insights from this study can be helpful in design of 2D metal-organic architectures consisted of linear rod-like organic ligands on solid surfaces.

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