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(G*) N-heterocyclic carbene adsorption and self-assembly on Au(111): Fine-tuning the binding mode

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Organic molecules capable of forming strongly bound self-assembled monolayers (SAMs) offer a promising route to surface modification and functionalization. Technological advances including the protection and stabilization of nanoparticles and the development of lab-on-chip sensors have been largely realized by the adsorption of alkanethiols. *N*-heterocyclic carbenes (NHCs) were recently introduced as alternative anchors in the preparation of SAMs on metal surfaces and may be superior to thiol-based systems. NHCs have important advantages compared to thiol-based systems, most notably their chemical tunability and ability to form strongly bound monolayers with improved stability. Given their novelty in the field of materials science, many fundamental properties of NHC-based SAMs are not well-understood, including factors that control the adsorption and self-assembly processes.

By means of scanning tunneling microscopy and further supplemented by *ab initio* (DFT) and Monte Carlo simulations, we investigate the mechanisms by which NHCs bind and self-assemble on Au(111). Our investigation demonstrates a critical dependence of the binding mode on NHC structure, surface coverage, and substrate temperature. The dependence on these factors arises due to the minimization of molecule-surface steric interactions, the production of Au adatoms by the effect of NHC adsorption on the underlying gold substrate, and the reactivity and stability of the ligand, respectively. The main effect on the adsorption process is a competition between upright attachment geometries and the formation of flat-lying bis-NHC-metal complexes. These species form a rich variety of self-assembled structures, including in particular a zig-zag lattice formed by adatom-bound NHCs and a non-porous chiral Kagome lattice containing trapped NHC monomers. These lattices are analyzed within our three-pronged methodology, providing valuable insights into molecule–molecule and molecule-substate interactions, as well as the role of surface modifications and on-surface chemical reactions in the formation of NHC SAMs. Efforts to understand these processes were crucial in advancing the chemistry and applications of thiol-based SAMs, and will similarly offer critical strategies for the design of upright NHC SAMs and their applications.

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