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Molecular-level study of N-heterocyclic carbenes for biosensing: orientation and self-assembly

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Self-assembled monolayers (SAMs) of organic molecules are extensively used to functionalize surfaces for a wide range of applications from medicine to nanophotonics. However, creating a SAM that is sufficiently stable has been a persistent problem. Although thiols have been the gold-standard for thirty years, N-heterocyclic carbenes (NHCs) have recently been used to create SAMs that are more thermally and chemically stable [1]. NHCs based on diisopropyl benzimidazolylidene (NHC^{iPr}) have also been integrated into biosensors [2]. The field of NHC-based material science is very new and the self-assembly mechanisms are still not well understood.

To provide a molecular-level perspective, we combine density functional theory (DFT) with scanning tunneling microscopy (STM) to study the self assembly of NHC^{iPr} on Au(111) at temperatures as low as 5K in ultra high vacuum (UHV). The isopropyl wing-tip groups of NHC^{iPr} play an important role in the self-assembly. They are responsible for both steric interaction with the surface and for stabilizing an ordered zig-zag lattice via intermolecular CH-pi hydrogen bonds. These NHCs are bound to adsorbed gold atoms (adatoms) extracted from terraces and from step edges, but unlike other systems that have been reported they are relatively immobile at 77K and their surface transport mechanism is largely dominated by a second phase. Through thermal annealing we induced conversion of the zig-zag lattice into flat-lying (NHC^{iPr})₂Au complexes. These complexes interact weakly with the surface and are highly mobile, yet they self-assemble into an ordered lattice when spatially constrained.

The discovery of two different NHC surface phases in this system is completely new. The first upright zig-zag phase can be readily functionalized and used in biosensors. The second phase of (NHC^{iPr})₂Au complexes exhibits intriguing instabilities that will be discussed. These results are a major step forward in understanding the mechanism for self-assembly of NHCs, a process which for thiols has taken thirty years to understand.

[1] C. M. Crudden, et. al, Nature Chemistry **6**, 409 (2014).
[2] C. M. Crudden, et. al, Nature Communications **7**, 12654 (2016).

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