Carbenes to tune 2D metal organic frameworks

Aliki Soufla,[a] *Anthoula C. Papageorgiou*[a]

[a]*Physical Chemistry Laboratory, Department of Chemistry, National and Kapodistrian University of Athens, Athens,15771,Greece*

e-mail: alikisoufla@chem.uoa.gr

Two-dimensional metal-organic frameworks (2D MOFs) have emerged as highly tunable materials with promising applications in catalysis, electronics, and nanotechnology.[1] However, controlling their surface properties through functionalization remains a significant challenge. We will present a strategy for the use of N-heterocyclic carbenes (NHCs) to fine-tune the electronic properties of 2D MOFs. While NHCs are widely studied for their role in catalytic metal surface functionalization for medical and luminescent applications, their integration into solid-state materials like MOFs remains underexplored.[2] Based on recent findings that demonstrate the reversible binding of prototypical NHCs to surface single-atom sites in a square planar coordination environment,[3] we propose to use the electron-donating capabilities of different NHC ligands as dopants of 2D-MOFs. In particular, we propose NHCs of varying electron-donating character in order to exemplary modulate the band structure and work function of a 2D MOF, namely of the semiconducting single layer $Cu_3(C_6O_6)$ on Cu(111) (figure 1).[4] A suitable experimental investigation under ultra-high vacuum (UHV) conditions to ensure atomically precise surfaces will be outlined. The structural and thermal stability of NHC-functionalized MOFs will be characterized using temperature-dependent scanning tunneling microscopy, while the band structure and work function will be evaluated through scanning tunneling spectroscopy and Kelvin-probe force microscopy. The outcomes of this research will provide critical insights into the design of flexible nanomaterials with optimized surface and electronic properties, offering broad implications for future applications in catalysis, electronics, and nanotechnology.

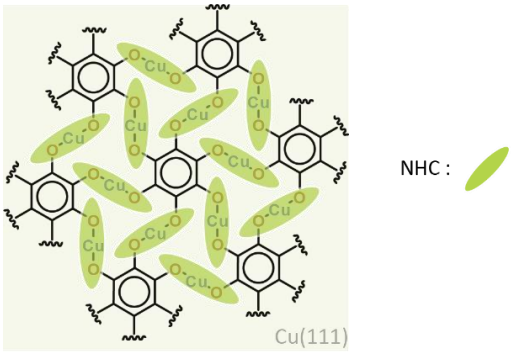

Figure 1. 2D MOF $Cu_3(C_6O_6)$ on Cu(111) functionalized with NHCs bonded to the MOF Cu atoms.

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