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Heterocyclic Carbenes for Tunable Functionalization of Oxide Surface.

N-Heterocyclic carbenes (NHCs) [1] exhibit excellent ligand properties as surface modifiers, owing to their structural diversity, tunable electronic properties, and strong affinity for a broad range of elements. These features make them highly attractive for applications in materials science and catalysis. [2] To fully harness the potential of NHCs in nanotechnology, it is essential to develop a fundamental understanding of their interactions with various metal oxide surfaces. While their behavior on metallic surfaces such as Cu, Ag, Pt, and Au has been extensively studied and rationally designed, synthesized, and analyzed, [2-5] their adsorption characteristics on oxidic supports remain less explored. First results showed that NHCs on oxidized copper surfaces are preferentially bound to oxygen atoms, [5] at variance from what is commonly observed in organometallic coordination complexes. The desorption of cyclic urea species promoted the reduction of copper oxide surfaces. [5] In this study, we investigate the adsorption behavior and electronic interactions of diverse NHCs on a range of metal oxide surfaces, spanning from ionic (MgO) or covalent (SiO2) large-gap oxides to small gap TiO2 and Cu2O. By means of hybrid DFT calculations we show how NHCs can bind either to oxygen or metal surface species. The charge state of the adsorbed molecules (almost neutral when bound to surface cations, positively charged when bound to oxygen) and the interfacial dipole moment are drastically different in the two cases. The preferential adsorption mode depends on the oxide electronic structure, as well as on the molecule electronic and steric features. Our findings pave the way for the rational design of NHC-based assemblies for tuning nanopatterned structures on oxide materials. [6]

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