

# Density functional studies of metal-organic interfaces: Corroles on Ag(111)

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Corroles are a class of heteroaromatic macrocycles that coordinate metal atoms in a formal oxidation state of +3. This is leveraged in a wide variety of applications including gas sensing [1], medical imaging [2] and catalysis [3].

These molecular systems have also sparked the interest of researchers in the field of surface science [4]. Here, corroles and related compounds were initially proposed as scaffolds for reactive metal ions to facilitate the growth of 2D-lattices [5]. However, it was shown that corroles are non-innocent (i.e. redox active) ligands [6]. We propose that this non-innocence offers the possibility of fine-tuning properties by changing chemical functionalization of the backbone. A distinguishing feature of free-base corroles is their acidity [7]. The loss of hydrogen to the Ag(111) surface has also been observed at temperatures of 240 K and higher [8].

We use dispersion-corrected Density Functional Theory-based approximations in a supercell approach to determine preferred adsorption sites and corresponding adsorption energies of free-base corroles and their metal complexes on Ag(111). The electronic structure is studied by means of bonding analysis while also generating theoretical spectroscopic data. Surface reactions and their kinetic barriers are modeled *in silico* to interpret and predict experimental results.

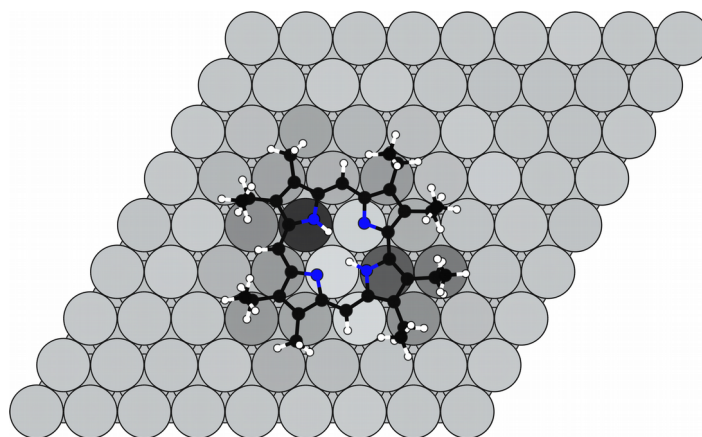


Figure: Corrugation of the Ag(111) surface due to adsorption of a substituted 2H-Corrole.

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