

Surface assisted cross-coupling of Pd- cyclometallated complexes on Ag(110).

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Cyclometallated complexes are good candidates as precursor molecules to build low-D carbon-based networks doped with metal atoms. Such nanostructures can be produced using a surface assisted, bottom-up approach since the molecules are thermally stable and can be sublimed in vacuum conditions. However, the few studies reported in literature [2,3] mainly refer to Ir(III)- and Pt(II)-containing complexes, of interest as light emitters, while relevant catalytic properties are foreseen using other metallic elements like Pd.

We report on the interaction of Ag(110) with Pd cyclometallated compounds [4,5]. The complex [(5-bromo-2-phenylpyridine)Pd(μ -Cl)]₂ is deposited on the surface at room temperature by sublimation in ultra-high vacuum. The thermal evolution of the system is followed by scanning tunnelling microscopy and X-ray photoemission spectroscopy, while the initial and final configurations are validated by ab-initio calculations. Our results demonstrate that the molecule dissociates due to the interaction with the surface and a cross coupling reaction between the two organic fragments occurs, leading to the surface assisted synthesis of diphenylbipyridine molecules. Such a process, occurring with low probability at RT, is thermally activated and competes with desorption. At variance with most cross-coupling reactions at surfaces reported in literature, in this case the reactants come from the dissociation of the same compound so that only one precursor is employed, leading to a simplified preparation protocol. The Br and Cl atoms dissociated from the molecule bind to the surface and promote an extended surface reconstruction upon annealing, which was not observed previously upon deposition of halogenated aromatic compounds.

References (if needed)

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