Dealkylation and Metallation of a Hydrocarbon in On-Surface Synthesis

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On-Surface Synthesis is established for the creation of extended, one- and twodimensional macromolecules by homo-coupling directly on a surface [1]. In comparison to classical solution based-chemistry, On-Surface Synthesis has a reduced parameter space (temperature, light) and currently focuses on developing reaction selectivity. Precursor design controls product formation. The build-up of non-stochastic hetero-coupled systems is highly desirable yet not achieved.

Here, we are studying with STM a picene derivative [2] as a precursor, named C_{12} -PicDI, adsorbed on Au (111). Imide moieties, which are reactive to metal ions, are attached to both ends (PicDI). Initially, the reactive end groups are passivated by weakly bond alkyl chains ($C_{12}H_{25}$). We demonstrate temperature-controlled removal of the alkyls and discuss the system evolution under varying experimental parameters. Alkyl byproducts thermally desorb from and only PicDIs remain on the surface. Selectively removing passivating alkyl groups through controlled heating activates the imide moieties, enabling subsequent metal ion coordination. This work demonstrates a crucial step toward realizing complex, designed heterostructures on surfaces [3].



Figure 1: Thermally activated metallation of a C₁₂-PicDI precursor

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