NC-AFM recognition of molecular adsorption and on-surface reaction of Si and triple bond containing molecule

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In this work we are focusing on identification of reactants and products of Cu(111) mediated on-surface reaction. We used Non-Contact Atomic Force Microscopy (NC-AFM) experiments and simulations with microscope tip modified by CO molecule [1] for this purpose: The reactant is adorbed trimethelsilyl molecule. Since non-planar parts of this molecule are flexible, an enhanced model [2] of frequently used Probe Particle code [3,4] and extensive density functional theory (DFT) calculations were employed to recognise the atomistic model of the reactant, and to understand the experimentally measured contrast. The resolved model shows an unforeseen binding of small, partially aromatic molecule to the copper surface. The examined reaction was one-shot desilylative homocoupling performed for the first time on Cu(111) surface and which resulted in diacetylene linked anthracene oligomers. The NC-AFM force measurement combined with theoretical calculations revealed the chemical nature at the centre of products anthracene unit [5].

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