Direct formation of C-C double and triple bonded structural motifs by on-surface dehalogenative homocoupling reactions

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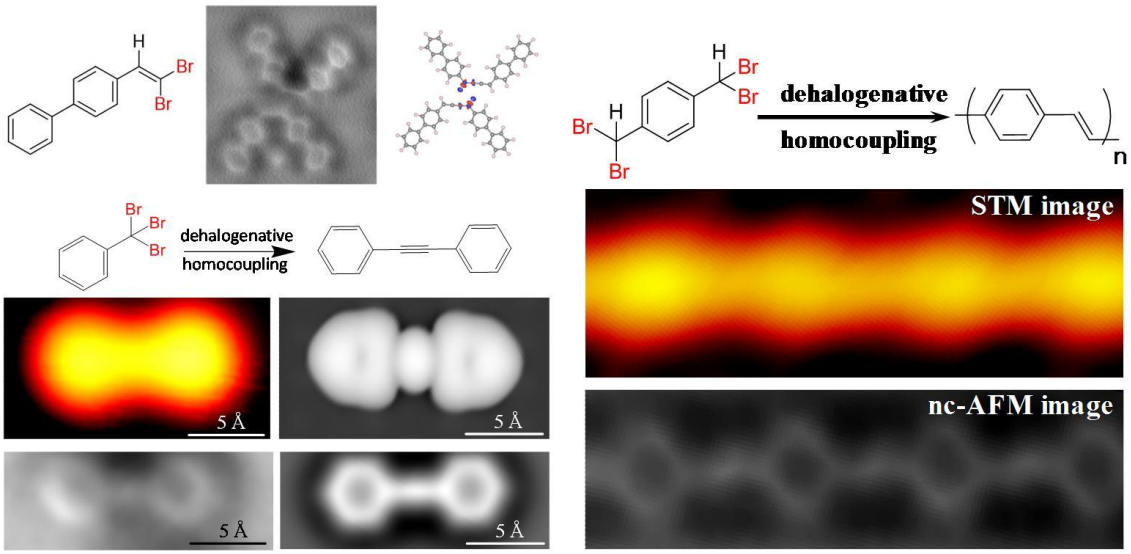
Recently, on-surface synthesis has aroused great attentions due to its fascinating potential in constructing novel nanostructures. In particular, C-C coupling between reactants by activation of predefined C-X groups (X stands for hydrogen or halogens) followed by the formation of new carbon-carbon bonds, represents one of the great choices for controllable fabrication of novel carbon nanostructures and low-dimensional carbon nanomaterials. So far, most of the halide precursors employed for dehalogenative homocouplings have only one halogen attached to a carbon atom. Herein, we designed and synthesized molecular precursors with gem-dibromomethyl/alkenyl gem-dibromides or tribromomethyl groups, by using the combinationof high-resolution scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) imaging and density functional theory calculations, we demonstrated that it is feasible to achieve the direct formation of C-C double or triple bonded structural motifs via on-surface dehalogenative homocoupling reactions [1-4]. Such studies provide an alternative route to the fabrication of emerging carbon nanostructures like carbyne, graphyne which involve the chemically vulnerable sp-hybridized carbons.

Keywords: scanning tunneling microscopy, non-contact atomic force microscopy, density functional theory, on-surface chemistry, dehalogenative C-C coupling



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