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Computational Study of Phenylacetylene Self-Assembly on Au(111) Surface[1] CHENGBO HAN, WENCHANG LU, JERRY BERNHOLC, NCSU, QING LI, MIGUEL FUENTES-CABRERA, HUMBERTO TERRONES, BOBBY SUMPTER, JIEYU YI, ZHENG GAI, ARTHUR BADDORF, PETRO MAKSYMOVYCH, MINGHU PAN, CNMS, ORNL, CENTER OF NANOPHASE MATERIALS SCIENCES, ORNL TEAM, NC STATE UNIVERSITY TEAM — The direct control over Phenyl-Acetylene (PA) self-assembly/disassembly on gold, achieved by carrier injection through an STM tip, is unprecedented. We discuss theoretical interpretation of PA structures observed on Au(111) by direct STM imaging in the preceding talk. We have examined 20 different adsorption geometries through first-principles calculations, simulated their STM images and compared them to the experimentally observed patterns. While weakly adsorbed PA prefers flat orientation on Au(111), the self-assembly leads to significant rearrangement of its adsorption structure. We obtain excellent agreement with the experimental data for a densely packed, ordered monolayer of vertically aligned but tilted styrene-derivative adsorption geometry, in which the acetylene tail is directly bonded to the surface. All the major features of the experimental STM image are reproduced by calculations, leading to unambiguous determination of the self-assembled structure [1]. We will also discuss the changes in adsorption energetics and molecular level alignment induced by the self-assembly process.

[1] Q. Li et al., ACS Nano, 6, 9267(2012)

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