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Visualizing Halogen Bonds in a Two-dimensional Supramolecular System

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Covalently bonded halogen ligands possess unusual charge distributions, attracting both electrophilic and nucleophilic molecular ligands to form halogen bonds. In many biochemical systems, halogen bonds and hydrogen bonds coexist. The interplay between halogen and hydrogen bonds has been actively studied in various three-dimensional bulk molecular co-crystals. It was found that halogen bonds could be complementary to hydrogen bonds due to their similar bond strength and dissimilar directionality. In those ensemble-averaging approaches, however, it was not possible to extract local information such as individual bond configurations and nano-level domain structures, which is a crucial part of supramolecular studies. In this study, we directly visualize the individual molecular configuration of a brominated molecule and the role of halogen bonds on Au(111) using scanning tunneling microscopy. The precise arrangement of observed molecular structures was reproduced by first-principle studies and explained in the context of halogen and hydrogen bonds. We discuss the distances and the strengths of the observed halogen bonds and hydrogen bonds, which are consistent with previous bulk data.

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