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Real-space identification of intermolecular bonding with atomic force microscopy

XIAOHUI QIU, National Center for Nanoscience and Technology, China

A covalent bond is a chemical bond that involves the sharing of electron pairs between atoms, whose formation and breaking result in chemical reactions and the production of new substances. Distinct from the covalent bond, the intermolecular interactions are often a vague concept elusive in experimental observations. Nevertheless, intermolecular interactions virtually affect all physical and chemical properties of substances in the condensed phases. The interactions between molecules, particularly the hydrogen bond, are responsible for the structural transformations and functions of biological molecules. Because most of the molecular characterization techniques are more sensitive to the covalent structures of the molecules, it remains a challenge to quantitatively study the weak interactions between molecules despite the tremendous efforts toward this goal. Here we report a real-space identification of the formation of hydrogen bonding between molecules adsorbed on metal substrate using a non-contact atomic force microscope (nc-AFM). The atomically resolved molecular structures with unprecedented details enable a precise determination of the characteristics of the hydrogen bond network, including bonding sites, orientations and lengths. The observed bond contrast was interpreted by ab initio density functional calculations that indicate the electron density contribution from the hybridized electronic state of hydrogen bond. Given the extensively discussion on the nature of hydrogen bonding and the recent redefinition by IUPAC, the observation of hydrogen bonding in real-space may be a stimulating evidence for theoretical chemistry. Meanwhile, the direct identification of local bonding configurations by nc-AFM would advance the understanding of intermolecular interactions in complex molecules with multiple active sites, offering complementary structural information essential for various applications in materials and biological sciences.