Abstract Submitted
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Atomic Force Tomography of a Nonplanar Molecule: Role of Lateral and Chemical Sample-Tip Interactions[1] XIANGHUA KONG, Ph. D candidate, WEI JI, Professor, PHYSICS DEPARTMENT, MCGILL TEAM, PHYSICS DEPARTMENT, RENMIN UNIVERSITY OF CHINA TEAM — Atomically identification of the molecular geometric structures is an important prerequisite to understand their chemical and electrical properties. TiOPc, a steric structure, gives rise to two adsorption configurations of TiOPc on Cu(111), namely O-dn and O-up. The roles of chemical specific interactions of different intramolecular atoms with the AFM tips were discussed at the submolecular level. For O-up, the molecular backbone of TiOPc is only visible out of a certain range from the center of the molecule, accompanied with significant dissipation signal. Theoretical calculation identifies such dissipation signal as the chemical attraction between the out-of-plane O in TiOPc and the Cu atoms behind the CO of a tip at a certain range of lateral distance between them. When they approach closer, the sample O repulses another O in the CO tip making it tilting strongly, which softens the tip and thus leads to even stronger O (sample) – Cu (tip) attraction. A direct demonstration of sample-tip electronic hybridization was manifested in the simpler O-dn case where an explicit wavefunction overlap between the tip O atom and the sample Ti atom. Given these results presented here, we anticipate that this method might be developed further generally useful in single-molecule chemistry and physics.

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