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Control the Au(111) Work Function by Substituted Aromatic Thiol Self-Assembled Monolayers

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Self-assembled monolayers (SAMs) prepared by aromatic thiols on gold surfaces have much larger potential for electronic device applications due to their electronic properties. In this study, the formation and structures of SAMs prepared by benzenethiol (BT), toluenethiol (TT), 2-fluorobenzenethiol (2-FBT), 3-fluorobenzenethiol (3-FBT), 4-fluorobenzenethiol (4-FBT), 4-chlorobenzenethiol (4-CBT), 4-fluorobenzenemethanethiol (4-FBMT), and 4-chlorobenzenemethanethiol (4-CBMT) on Au(111) were examined using scanning tunneling microscopy (STM) and Kelvin probe (KP) to explore the structure and electronic interface properties of eight differently substituted aromatic thiol SAMs on Au(111). And these values are compared with gas phase dipole moments computed by quantum chemical calculations for individual thiol molecules. It was revealed that all eight thiol-molecules form uniform SAMs on Au(111) at 75°C compared to lower solution temperature by STM observation. The work function change obtained in the KP measurements and calculated molecular dipole moments have the linear relationship while the 4-FBMT and 4-CBMT deviate from this tendency.

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