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### **Roles in Modulation of Molecular Structures on Metal Surfaces**

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We studied the adsorption of organic molecules, their growth behavior, and their physical properties on silver and gold surfaces at the single molecule or sub-molecular scale by using low-temperature scanning tunneling microscopes. Combined with low energy electron diffraction and first-principles density functional theory calculations, the key parameters in modulating molecular structures on metals are analyzed. It is found that the alkyl chains of quinacridone derivatives (QA) determine the orientation of molecular overlayers on an Ag(110) substrate. The interaction of QA and the Ag substrate is primarily due to chemical bonding of oxygen to specific positions at the silver substrate, determining the molecular orientation and preferred adsorption site. However, the intermolecular arrangement can be adjusted via the length of attached alkyl chains. We are thus able to fabricate uniform QA films with very well controlled physical properties. Furthermore, by thermal and chemical control, we are able to self-assemble three dimensional molecular nanostructures, e.g. ordered PTCDA structures exclusively on flat Ag(111) facets, or DMe-DCNQI structures exclusively on stepped Ag(221) facets. It is demonstrated that bonding, the key factor for selectivity, occurs via the end-atoms, while the molecule's mid-region arches away from the substrate. Theoretical results, obtained by high-level theory, are consistent with the experimental observations, which have previously been interpreted in terms of bonding through the mid-region.

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