## Surface Strain Mediated Dipole Alignment of CIAIPc on Au(111)/mica

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Scheme of an organic FET. TCNQ on Cu, organic/metal electrode interface. Nature Chemistry 2, 344 (2010)



Substrate Effects on the Order/ disorder Packing Nature Physics 5, 153 (2009) ML 0.0 1 2 3 4 5 GaCIPc/Cu(111)







Monolayer CIAIPc on Au(111) and Ag(111) Coverage-dependent work function Phys. Rev. B,87, 085205, (2013) Phys. Rev. Lett, 106, 156102 (2012)



Non-planar Dipole-PhthalocyanineOrganic molecular beam epitaxial (OMBE)Chloride Aluminum Pc (CIAIPc )Characterized by STMUltra-high vacuum low temperature scanning tunneling microscopy









Figure 1. (A)Unidirectional reconstruction of Au(111) on mica;(B) herringbone reconstruction of Au(111) single crystal; (C) ~0.9 ML CIAIPc molecules on the Au(111) single crystal; atomically resolved STM image of the FCC and HCP region on Au(111)/mica (D) and Au(111) single crystal (E); The linear packing structure of CIAIPc along the stripes of the Au(111)/mica reconstruction.



Concla	usion		
CIAIPc	Au(111)/mica 0.6ML	Au(111)/mica 0.9ML	Au(111) Single Crystal 0.9ML
Cl-up	~60%	~50%	~99%
Cl-down	~40%	~50%	~1%
Up-down 0-4	0	0	0
1-3	0	0.2%	0
2-2	~71%	~91%	0
3-1	~29%	~8.8%	0.3%
4-0	0	0	99.7%
Figure 3. The mo	lecular ordering and di	ipole ordering of CIAIPc	on Au(111)/mica and the

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Au(111) single crystal surface. The dipole alignment within each unit cell (four neighboring CIAIPc molecules) on different surface; and under different coverage is summarized.

**1.74%** increase of lattice constant along [1-10] comparing with the herringbone reconstructed Au(111)

Owhere intermolecular repulsion will be caused for identically aligned CIAIPc on Au(111)/mica;

□ Unique local ordering of dipole alignment comprising of one Cl-up and one Cl-down ClAIPc within one unit cell minimized the repulsion dramatically and stabilized the superstructure

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Figure 2. (A) Molecularly resolved STM image of CIAIPc on Au(111) single crystal, the VOPc molecules adopt unidirectional CI-up orientation; (B) ~0.5 ML CIAIPc on the Au(111)/mica surface, four-row stripes are formed within which the CIAIPc alternatively orientated with CI-up and CI-down configurations; (C) ~1ML CIAIPc molecules on Au(111)/mica surface, an alternative packing within the four-rows is preserved; their corresponding packing structure is demonstrated below in (D), (E) and (F) respectively; The proposed model of the formation of the four-row molecular stripes within one unit cell of the Au(111)/mica is proposed below, which indicates the epitaxial adsorption.