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Self-assemble of polar pyrene towards 1D and 2D ferroelectric array

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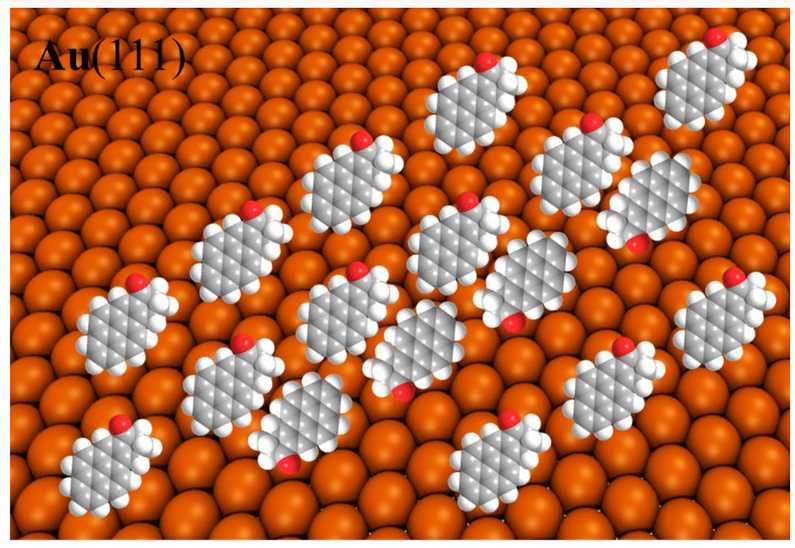
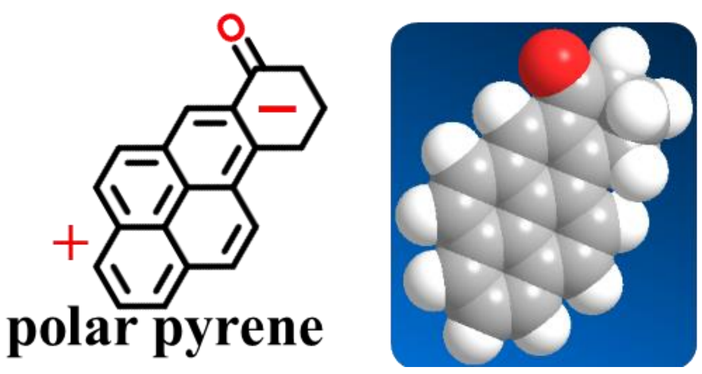
Abstract

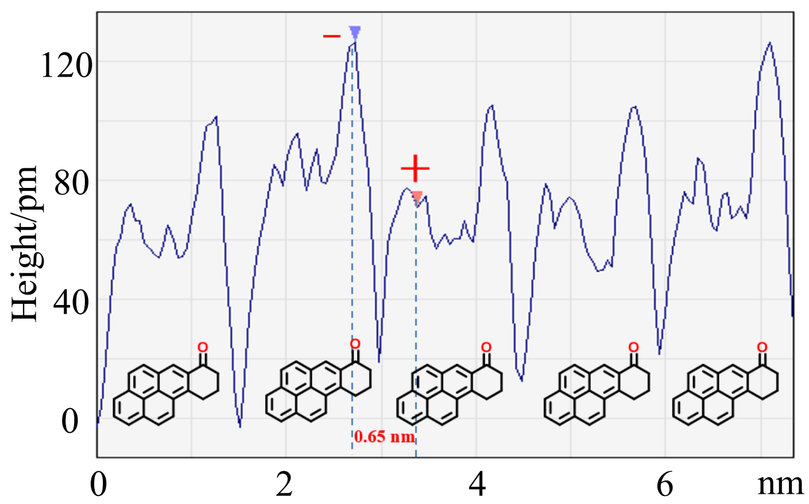
Ferroelectric materials have shown great promise in nonvolatile random access memories, capacitors, sensors, micro-actuators, and optical devices.[2] However, challenges are still need to be answered in order to manipulate single molecules into ferroelectric ordered array on surface. In this work, we demonstrate the reliable manipulation of polar pyrene precursors towards 1D wires and 2D ordered array. The proposed nature of 1D ferroelectric molecular wires of pyrene molecules on Au(111) is mainly governed by dipole-dipole interaction. More importantly, the intermolecular interaction via hydrogen bond is the key ingredient to generate the aforementioned structure into two dimensional ferroelectric ordered array.

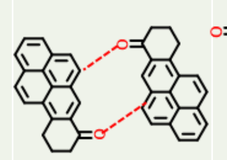
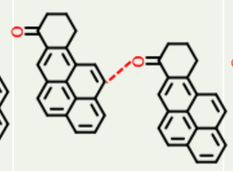
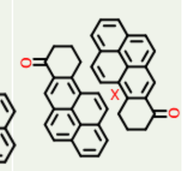


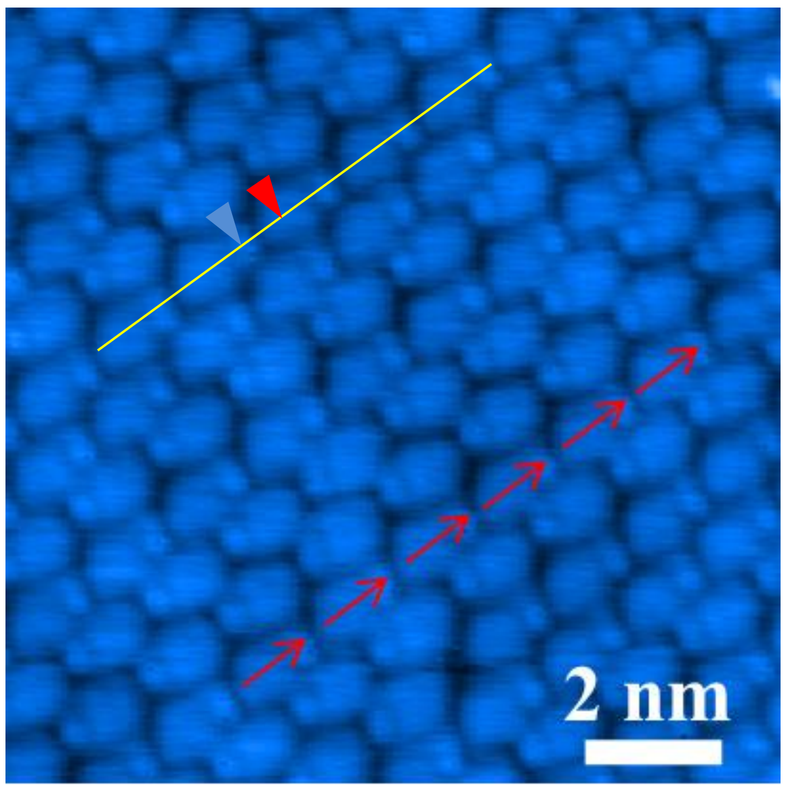
1D & 2D ferroelectronic molecular array

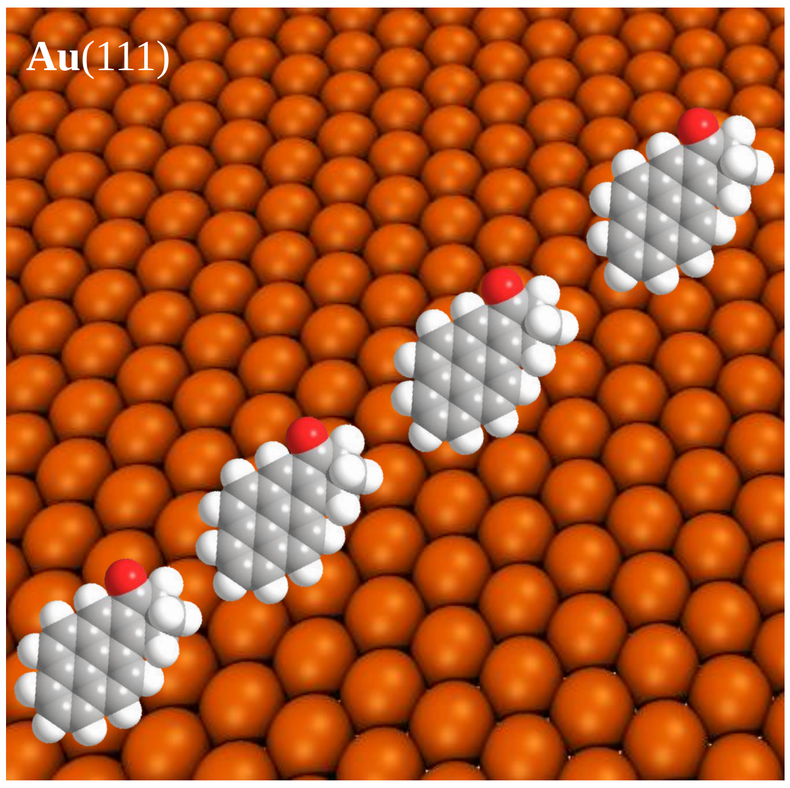
Results and Discussion





Hydrogen bond	2	1	0
Distance /nm	1.00	0.84	0.73
Molecular interaction			





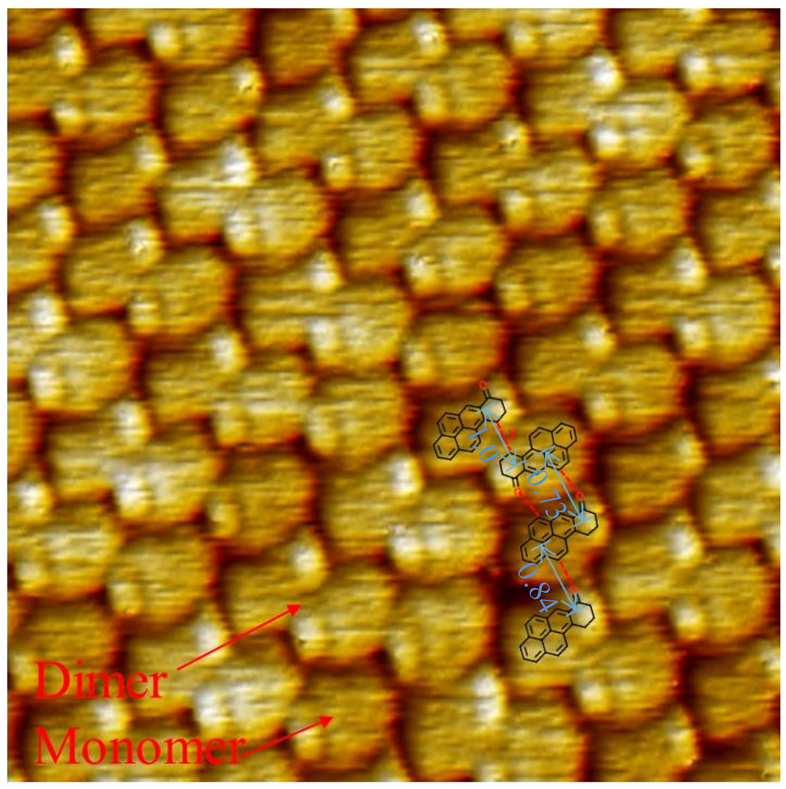


Fig.1 Constant current STM image reveals the molecular arrangement of polar pyrene on Au(111). V_{Tip}=-2.0 V, 72.6 pA and 77K.

Fig.2 The diagram illustrates self-assembly of polar pyrene to 1D ferroelectronic molecular wires driven by dipole-dipole interaction.

Fig.3 The evolution of 1D wires into 2D ferroelectric ordered array induced by hydrogen bond.

Conclusion and Outlook

In conclusion, we demonstrate for the first time the polar pyrene conversion from 1D molecular wires to 2D ferroelectric array on Au(111). These molecular arrangement can be realized due to intermolecular dipole-dipole interaction in combination with the hydrogen bond. The next goal is to investigate in great detailed the self-assembly mechanism of molecular array from the aspect of molecular coverage and the substrate effect. In addition, theoretical support based on the density functional theory will be employed to understand the nature of cooperativity effect of pyrene molecule on surfaces.

References

[1] D. Wang, Arramel, X. He, A. T. S. Wee, *in preparation*, **2017**.

[2] A. E. Baber, S. C. Jensen, E. C. H. Sykes, *J. Am. Chem. Soc.* **2007**, *129*, 6368-6369.

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