Linear array of cesium atoms assisted by uracil molecules on Au(111)

Electronic supporting information

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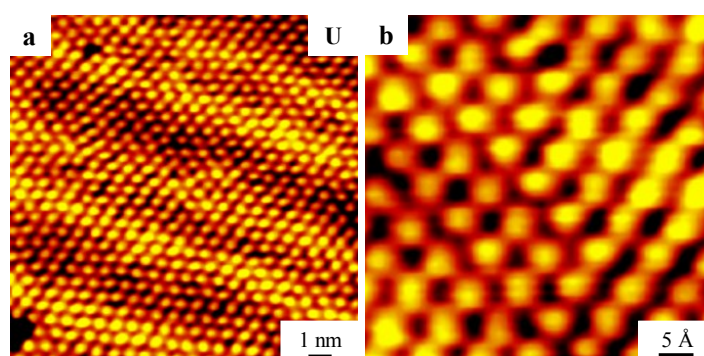
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Figure S1. (a) Large-scale and (b) close-up STM image of the self-assembled close-packed structure of U molecules.
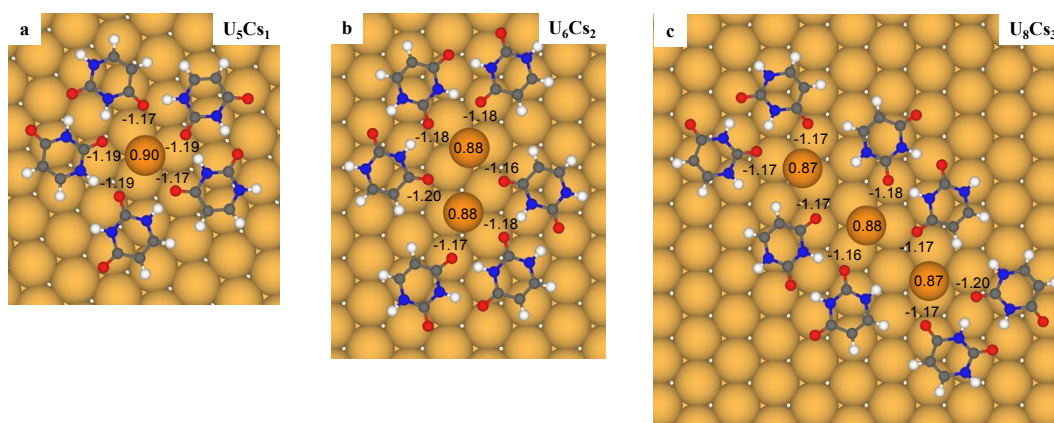

Figure S2. Bader charge analysis quantitatively shows the positively charged Cs atoms and negatively charged O atoms in the (a) U_5Cs_1, (b) U_6Cs_2 and (c) U_8Cs_3 metal-organic motifs.
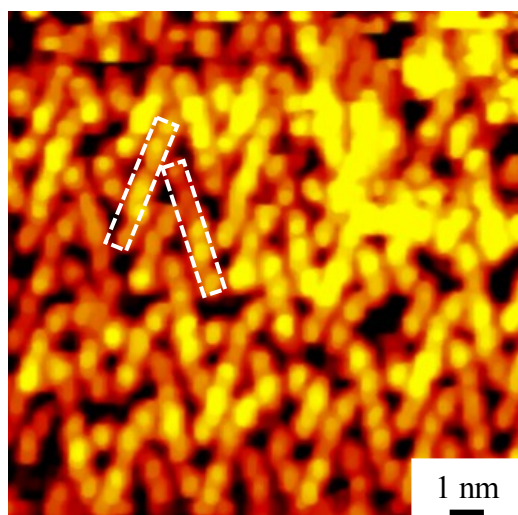
Figure S3. The STM image showing the network structure by further depositing Cs atoms on U_8Cs_4-precovered Au(111) surface and followed by annealing at 370 K. The white rectangles highlight the metal-organic motifs in which more than four Cs cations arraying linearly that could not be distinguished obviously.

Methods

All STM experiments were performed in a UHV chamber (base pressure 1×10^{-10} mbar) equipped with a variable-temperature, fast-scanning "Aarhus-type" STM using electrochemically etched W tips purchased from SPECS,[1,2] a molecular evaporator and an e-beam evaporator, and other standard instrumentation for sample preparation. The Au(111) substrate was prepared by several cycles of 1.5 keV Ar^+ sputtering followed by annealing to 800 K for 15 min, resulting in clean and flat terraces separated by monatomic steps. The Uracil molecules (purchased from Sigma-Aldrich (purity > 99%) were loaded into a glass crucible in the molecular evaporator. After a thorough degassing, the U molecules were deposited at 370 K by thermal sublimation. The alkali metal cesium was evaporated from Alvasource (from Alvatec) *via* conventional resistance heating after fully degassing. The sample was thereafter transferred within the UHV chamber to the STM, where measurements were carried out at ~150 K. All of the STM images were further smoothed to eliminate noises. Scanning conditions: It = 0.5~0.8 nA, Vt = ~ 1200 mV.

The calculations were performed in the framework of DFT by using the Vienna *ab initio* simulation package (VASP).[3,4] The projector-augmented wave method was used to describe the interaction between ions and electrons;[5,6] the Perdew-Burke-Ernzerhof generalized gradient approximation exchange-correlation functional was employed,[7] and van der Waals interactions were included using the dispersion-corrected DFT-D3 method of Grimme[8] for the calculations when including the gold surface. The atomic structures were relaxed using the conjugate gradient algorithm scheme as implemented in the VASP code until the forces on all unconstrained atoms were ≤ 0.03 eV/Å.

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