

## Supplementary Materials for

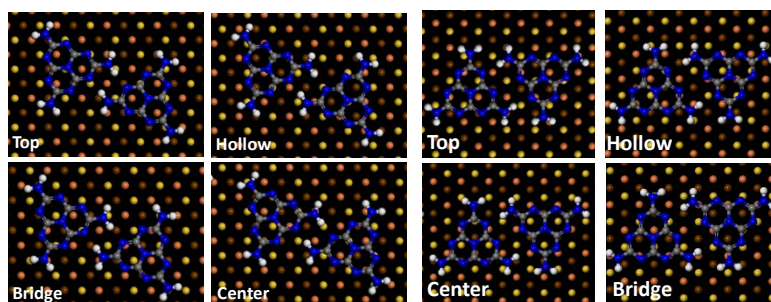
### Self-assembly of Melem on Au(111) and Ag(111): the origin of two different hydrogen bonding configurations

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	Top	Bridge	Center	Hollow
Motif-1	-761.72 eV	-761.64 eV	-761.66 eV	-761.66 eV
Motif-2	-761.50 eV	-761.37 eV	-761.47 eV	-761.33 eV

Fig. S1 The different sites of Motif-1 and Motif-2 on Au(111) in the upper figure, and their respective energies are shown in the lower table.

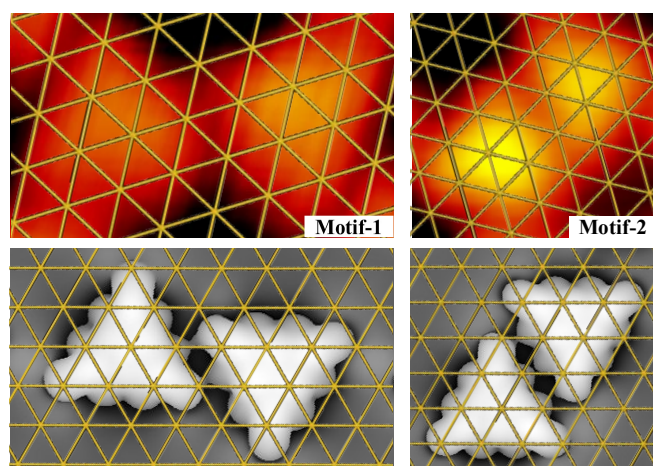


Fig. S2 The experimental STM images (top) and the Tersoff-Hamann STM simulations (below) of Motif-1 and Motif-2 on Au(111), where the lattices of the first Au(111) layer are indicated with grids.

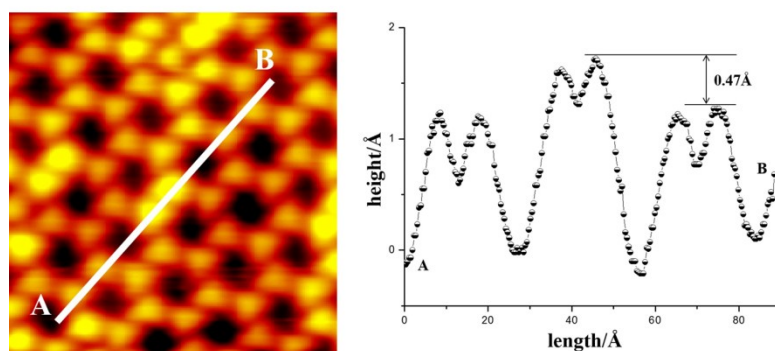
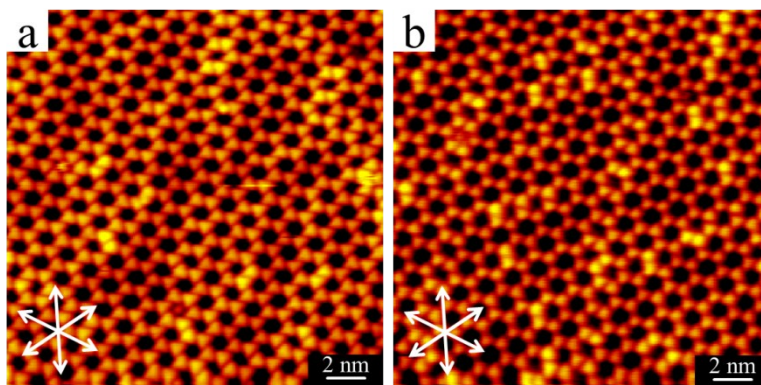


Fig. S3 Line profile across dim and bright dimer motifs, where the corresponding STM image and the position of the line profile is indicated in the left image.



Temperature	300K	350K	450K
Bright dimers			
Isolated dimers	22%	38%	28%
Aggregates of dimers	78%	62%	72%

Fig. S4 (a) and (b) STM images showing melem molecules on Au(111) surface at 350K and 450K, respectively. The distribution of dimer is shown in the lower table at different temperatures.

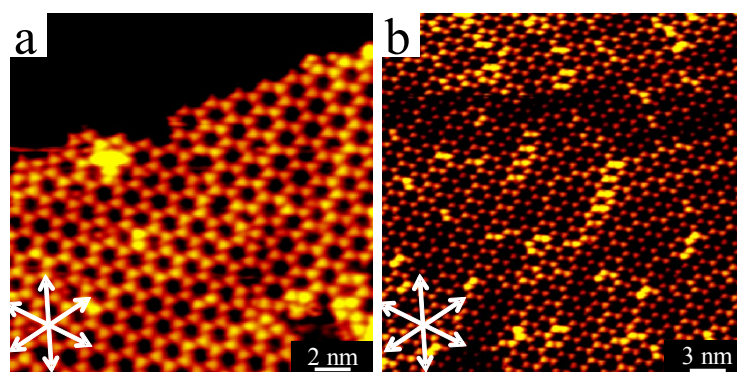
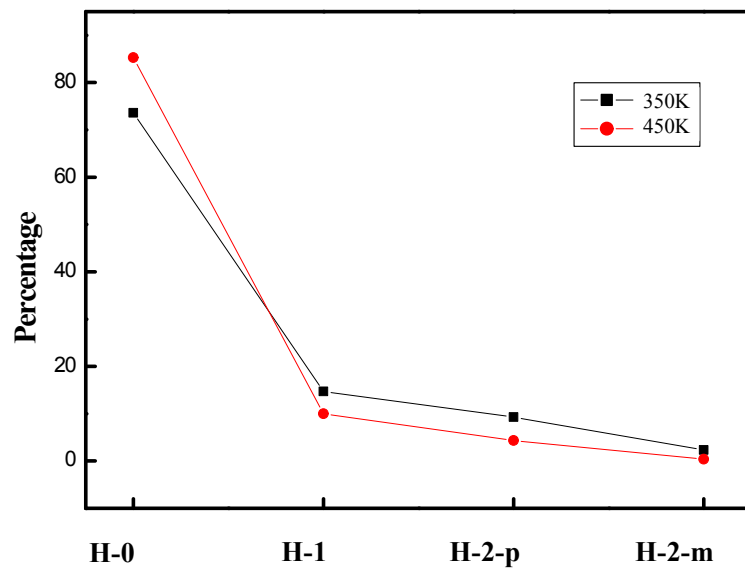


Fig. S5 (a) and (b) STM images showing melem molecules on Au(111) surface at different coverage. The proportion of bright dimers in (a) 0.2 ML is 2%, and (b) 0.5 ML of 3%



**Fig. S6 A** statistical distribution of the different hexamers observed on Au(111) at 350K and 450K.