Electronic Supplementary Material (ESI) for Nanoscale Advances.

ELECTRONIC SUPPLEMENRATY MATERIAL

TO

Thermally induced intra-molecular transformation and metalation of free-base porphyrin on Au(111) surface steered by surface confinement and ad-atoms

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Supplementary figures

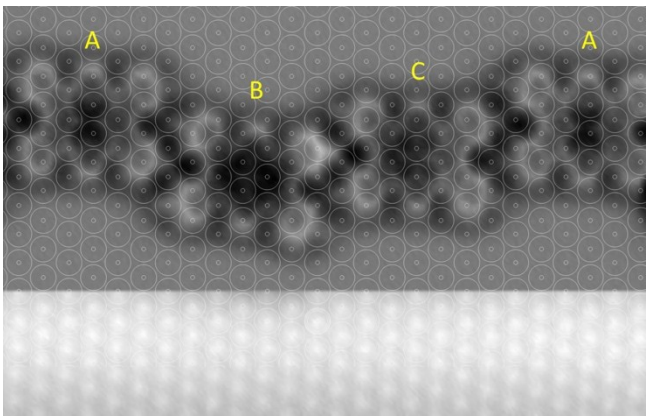

Fig. S1 High-resolution AFM image of A, B, C 2H-4FPP molecules and atomic resolution of Au(111) substrate. For atomic resolution of substrate, the tip was approached 400 pm towards the sample. The lattice of Au(111) surface is extended to the scanned area for atomic registration of A, B and C molecules adsorption site.

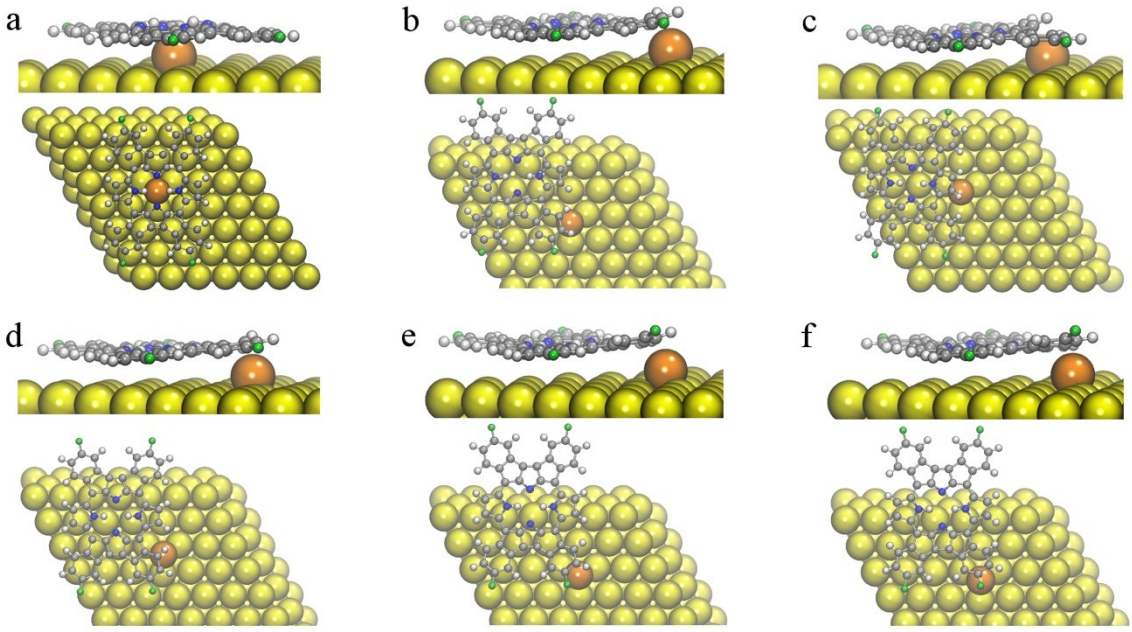

Fig. S2 Side- and top-view of 2H-4FPP on Au(111) with pre-adsorbed Au adatom (cf., Table 2): 1 (a); 34 (b); 2 (c); 3 (d); 45 (e); 5 (f). Gold atoms are shown in yellow (Au slab) and orange (adatom), C in grey, N in blue, F in green, and H in white.

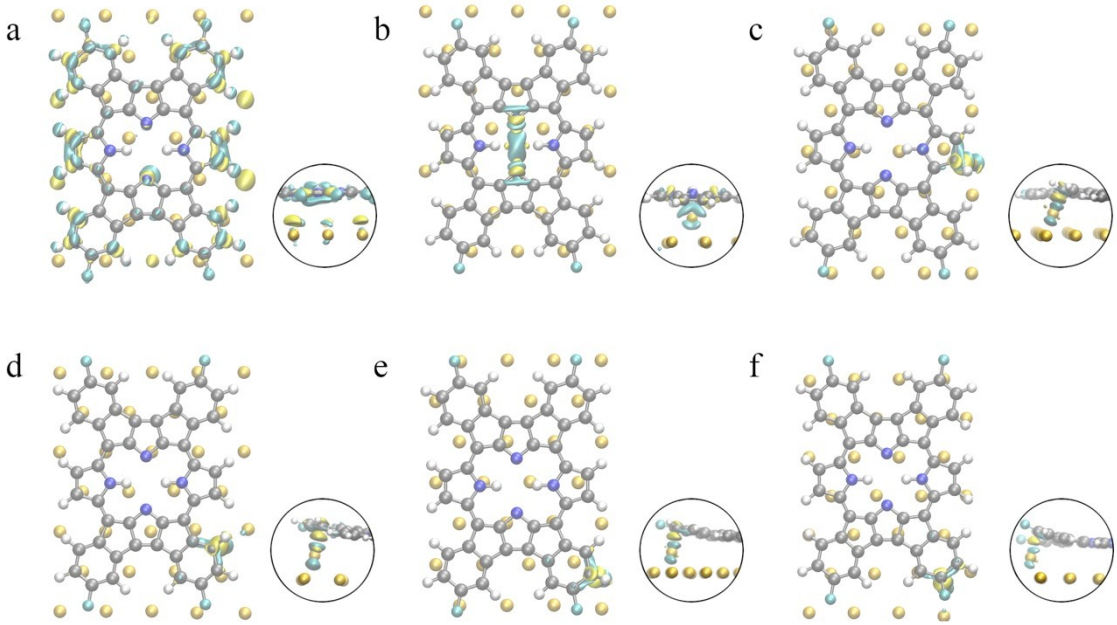

Fig. S3 Top- and side-view of surfaces of constant electron density difference plotted at ±0.02 eÅ^{-3} for 2H-4FPP on the bare Au(111) surface (a); and on Au(111) with pre-adsorbed Au adatom: 1 (b); 2 (c); 3 (d); 4 (e); 5 (f). Cf., Table 2.

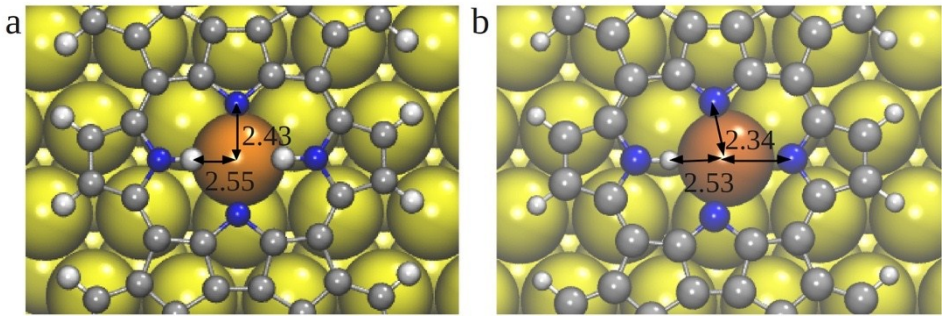

Fig. S4 Top-view of the 2H-4FPP on Au(111) with pre-adsorbed Au adatom and the Au-(H)N bond-lengths (in Å) indicated: (a) intact molecule; (b) molecule with the central H atom removed.