Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

Template-Controlled Sonogashira Cross-Coupling Reactions on a Au(111) Surface

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Contents

Reaction products formed out of a mixture of ***B1*** and ***A*** on Au(111) without template.

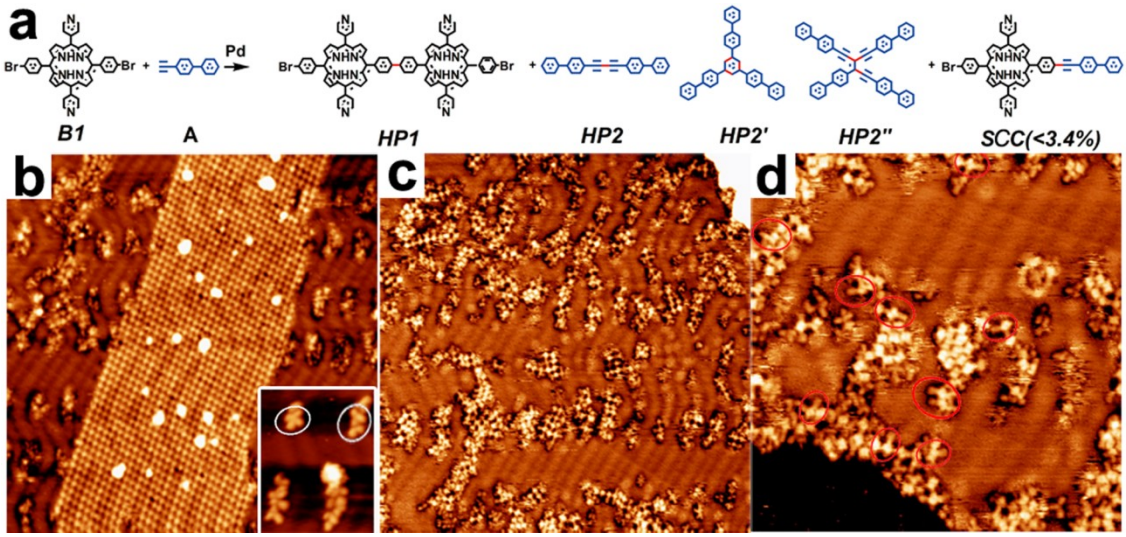

Figure S1 (a) Reaction products of a mixture of ***B1*** and ***A*** without template. STM images of Pd catalyzed reactions of ***B1*** and ***A*** on a Au(111) surface without template: (b) at room temperature (90×90 nm^2); inset shows a zoom-in area containing **HP2**, **HP2'** and **HP2''**, as indicating by white ellipse. (c) after annealing to 120°C (90×90 nm^2); (d) a zoom-in STM image after annealing to 120°C with SCC products indicated by red ellipse (40×40 nm^2).

SSC products formed with stepwise-increased dosage of ***A*** with ***T1***.

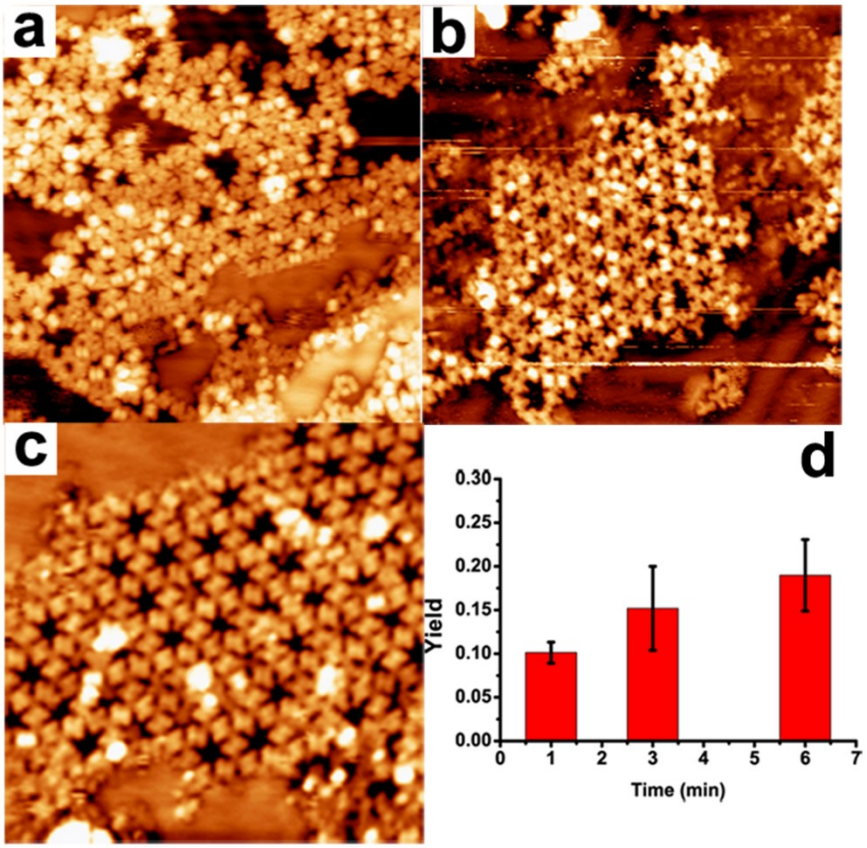

Figure S2 STM images of a stepwise dosing ***A*** onto ***T1*** with a dosage of (a) 1 minute (40 × 40 nm^2); (b) 3 minutes (40 × 40 nm^2) and (c) 6 minutes (23 × 23 nm^2) after annealing to 90°C in the presence of Pd;(d) yields of SCC products against the dosing time of ***A***.

Homo-coupled dimers of ***B1*** after annealing ***A*** and ***T2*** to 140°C

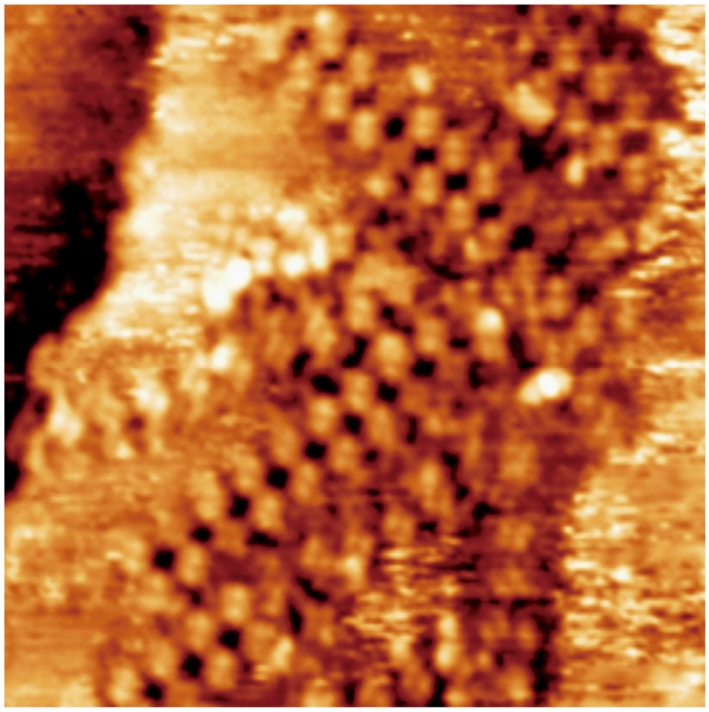

Figure S3 STM topograph showing ***B1*** formed via Ullmann coupling after annealing the sample of ***A*** with ***T2*** to 140°C (33×33nm^2).

After annealing the sample of ***A*** with ***T2*** to 140°C, the double-row ladder structures formed. The distance between the neighboring ***B1*** molecules perpendicular to the chain amounts ~1.78nm, evidencing a covalent bond formed between two ***B1*** molecules. Few SCC products were observed. Therefore, homo-coupling of ***B1*** is more favored at this annealing temperature.

High yield of SSC of ***A*** with ***T3***.

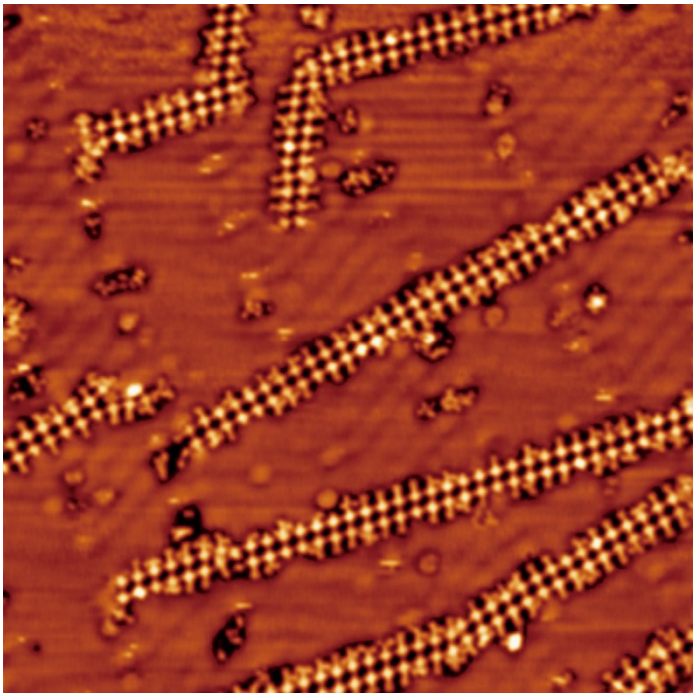

Figure S4 A large-scale STM topograph showing nearly all reaction sites on ***T3*** are cross-coupled to ***A*** after annealing to 170°C(75×75 nm^2).