Electronic Supplementary Material (ESI) for Analyst.

Electrochemically activated carbon−halogen bond cleavage and C-C coupling monitored by in situ shell-isolated nanoparticle-enhanced Raman spectroscopy

Chen-Chen Jiang, Xiao-Chong Li, Jian-Ang Fan, Jia-Ying Fu, Xu-Nan Huang-Fu, Jia-Jie Li, Ju-Fang Zheng, Xiao-Shun Zhou*, Ya-Hao Wang*

Key Laboratory of the Ministry of Education for Advanced Catalysis Materials, Institute of Physical Chemistry, Zhejiang Normal University, Jinhua 321004, China

* Corresponding authors
E-mails: xszhou@zjnu.edu.cn, yahaowang@zjnu.edu.cm

Supplementary Figures

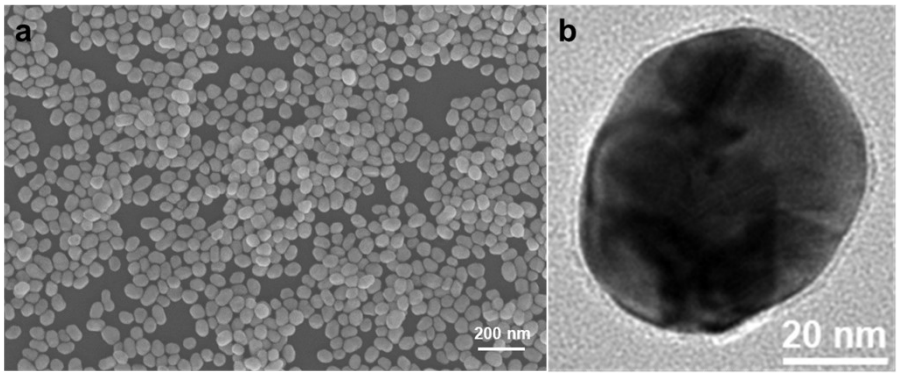

Fig. S1 SEM (a) and TEM (b) images of prepared 55 nm Au@ ca. 2 nm SiO_2 nanoparticles (SHINs).

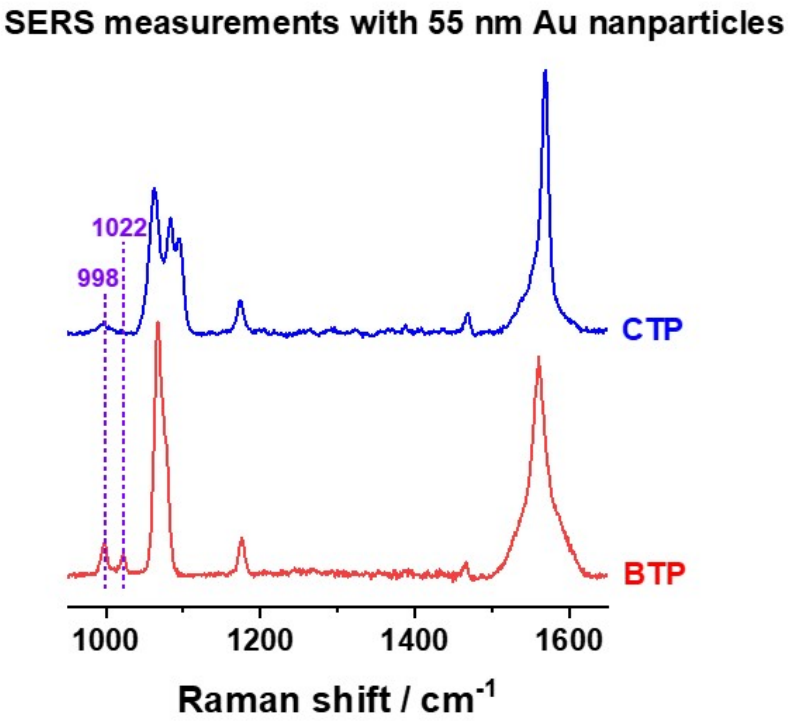

Fig. S2 SERS spectra of CTP and BTP on Au electrode. Notably, the bands at 998 (β_{CC}) and 1022 (β_{CH}) cm^{-1} are the characteristic features of TP generated by the plasmonic hot electron induced reaction .

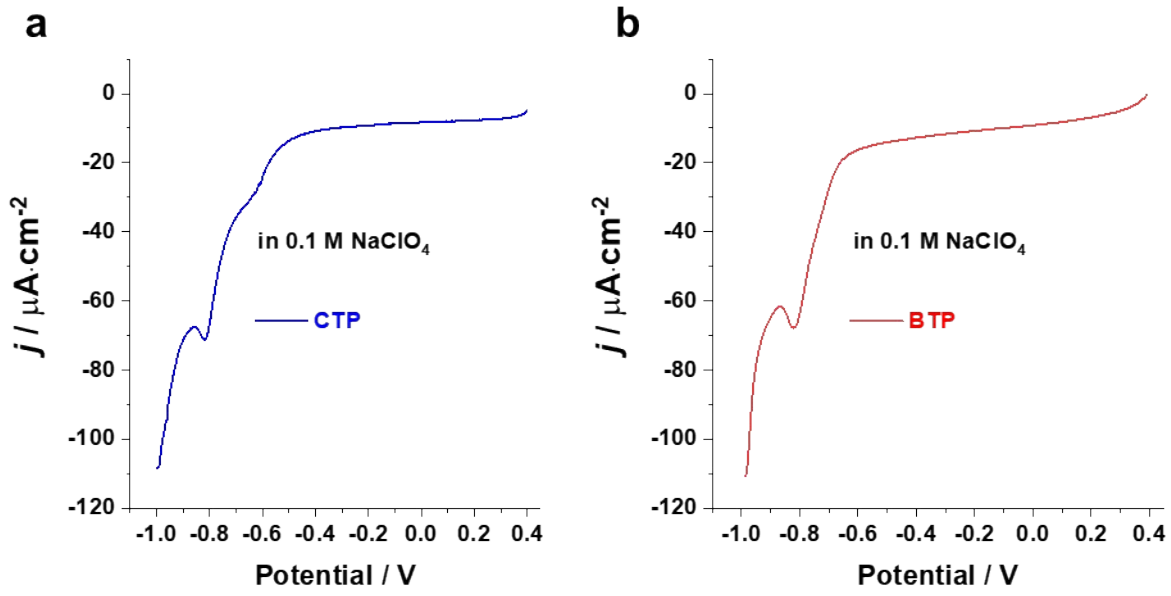

Fig. S3 The LSVs of CTP (a) and BTP (b) on smooth Au electrode in 0.1 M $NaClO_4$ (pH = 7) with a scan rate of 100 mV/s.

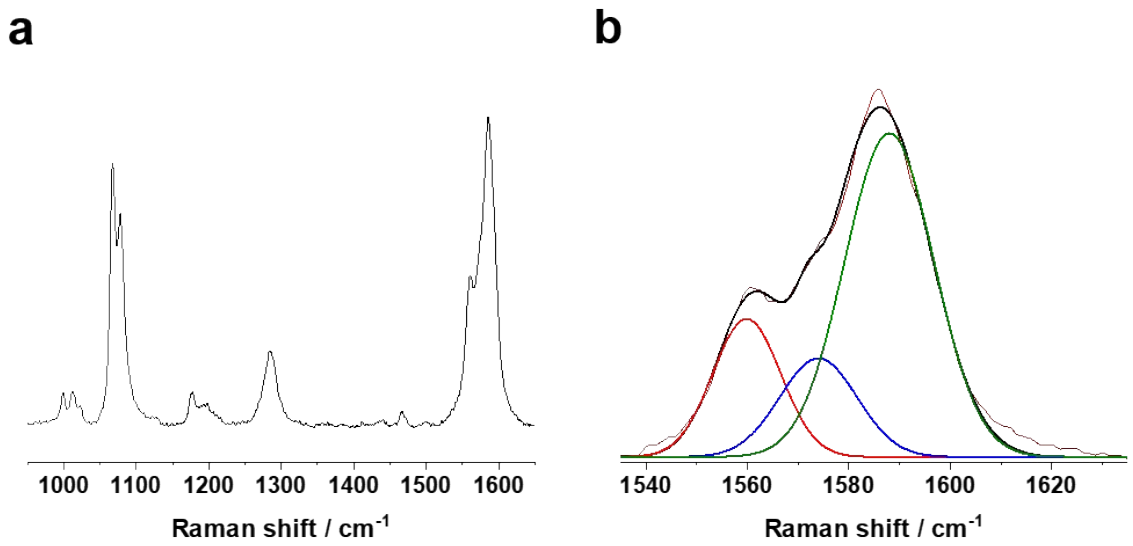

Fig. S4 (a) SHINERS spectrum of smooth Au electrode assembled molecules in a mixed solution containing 1/3 mM BTP + 1/3 mM TP + 1/3 mM BPDT. (b) The specific spectrum of ν(CC) with Gaussian peaks fitting for BTP(red), TP (blue line) and BPDT (green line). The derived peak area ratio is 1:1:3.8 for BTP:TP:BPDT, similar to that in the reported SERS measurements. [1] These differences are taken into account for calculating the relative concentration of the three components during the electroreductive dehalogenation process of aryl halide.

As these molecules with similar structures have the same anchoring group of -SH, we simply regard the composition of the monolayers is similar to that in the mixed solution, despite the substitution effect should modify the Au-S bond strength and molecular orientation. The advantage using the mixed monolayers is that their Raman spectra could be obtained in the same SERS hotspot to determinate the cross-section difference. A ratio of 1:3.8 (TP: BPDT) is found similar to 1:3.5 and 1:4.2 in the reported SERS measurements using the individual SERS spectra of BTP, TP and BPDT to determinate the ratio of SERS cross section of aromatic ν(CC) stretching modes.[1]

References

[1] Y. Li, Y. Hu, F. Shi, H. Li, W. Xie, J. Chen, C−H arylation on nickel nanoparticles nonitored by in situ surface-enhanced Raman spectroscopy, Angew. Chem.,Int. Ed., 58 (2019) 9049-9053.