

# Supporting Information

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## In-situ STM visualization of molecular structural evolution during electrochemical oxidation coupling of *para*-Aminothiophenol on Au(111)

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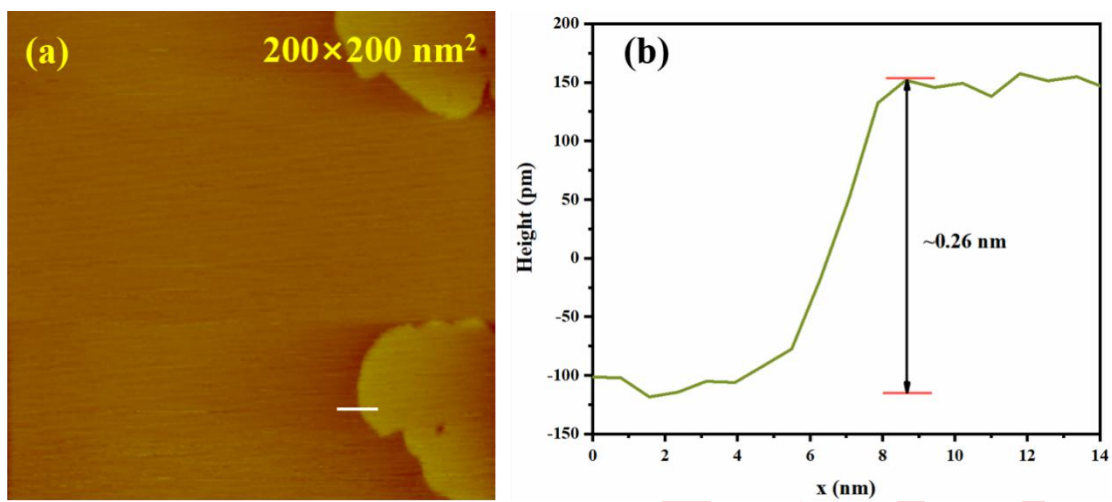
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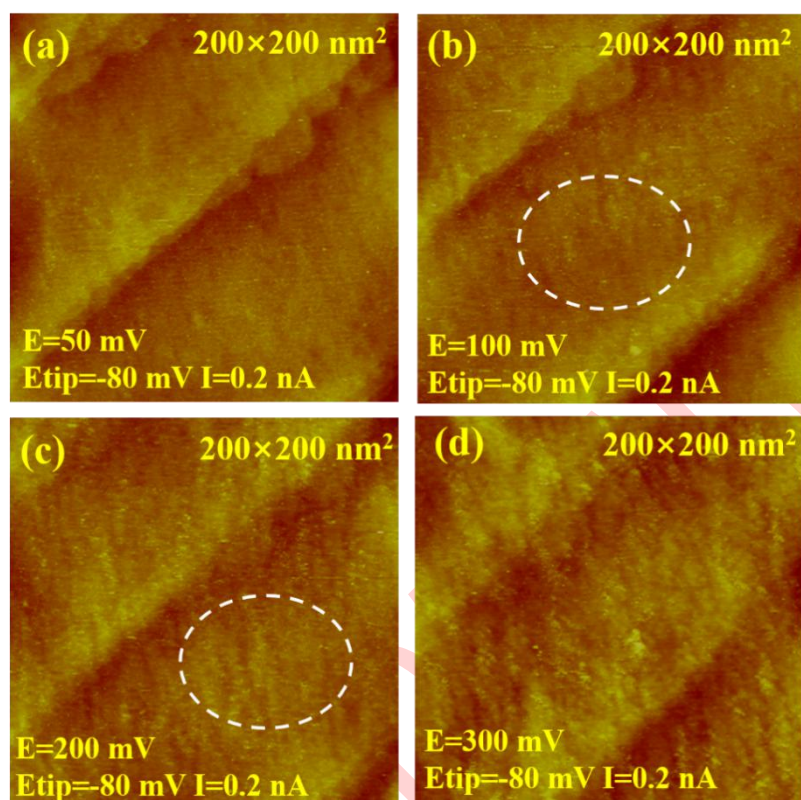
<sup>†</sup>These authors are contributed equally to this work.

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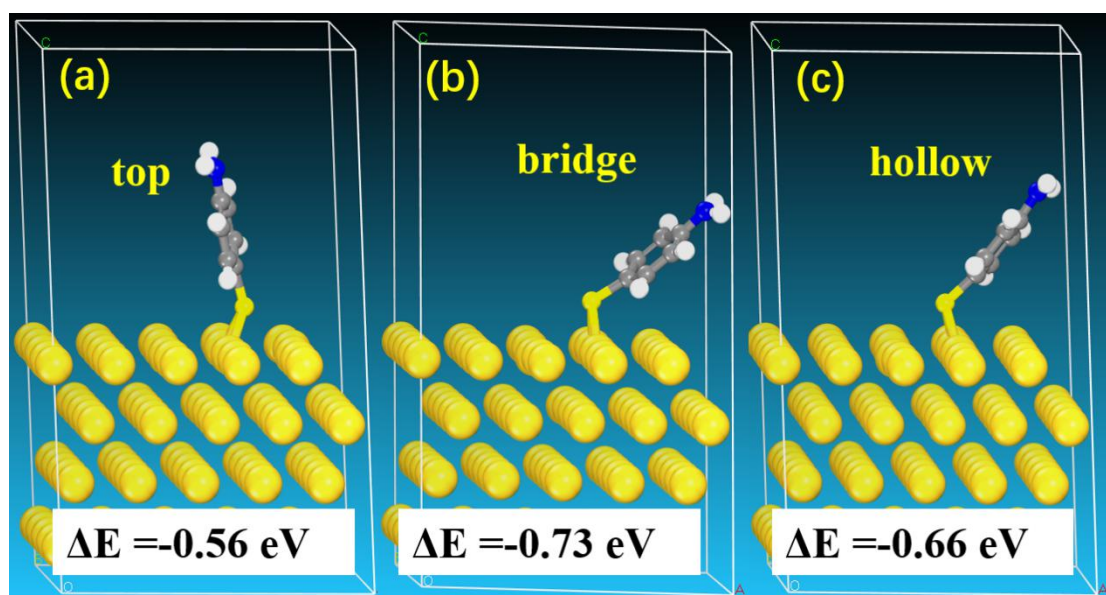
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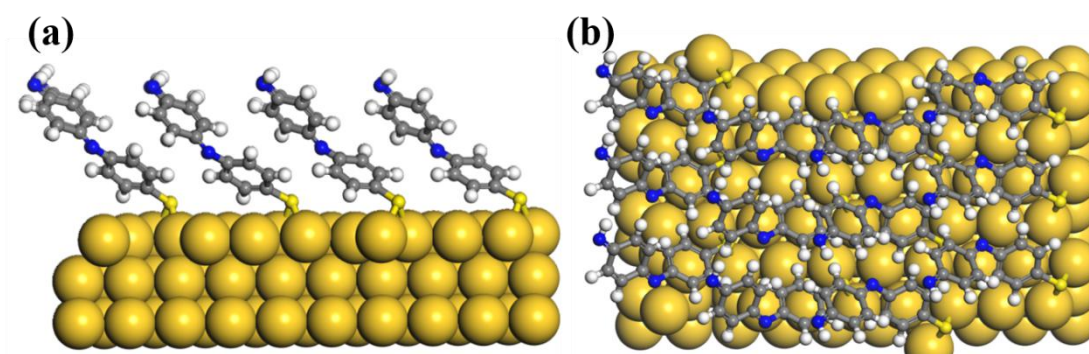
**Fig. S1** (a) EC-STM image of bare Au(111) surface and (b) measured step height.



**Fig. S2** STM characterization of Au(111)-PATP in the potential range of 50 to 300 mV. The sample potentials are (a) 50 mV, (b) 100 mV, (c) 200 mV, (d) 300 mV, respectively. Tunneling conditions: E<sub>tip</sub> = -80 mV, and I<sub>t</sub> = 0.2 nA.



**Fig. S3** Schematic representation of PATP adsorption at different sites of Au(111). (a) top site, (b) bridge site, (c) hollow site.  $\Delta E$  is the magnitude of adsorption energy of PATP adsorption at different sites.



**Fig. S4** Optimized structure of high coverage NPQD molecules adsorbed on an Au(111) surface in a  $\sqrt{3} \times 4\sqrt{6}$  structure, (a) side view and (b) top view.

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