

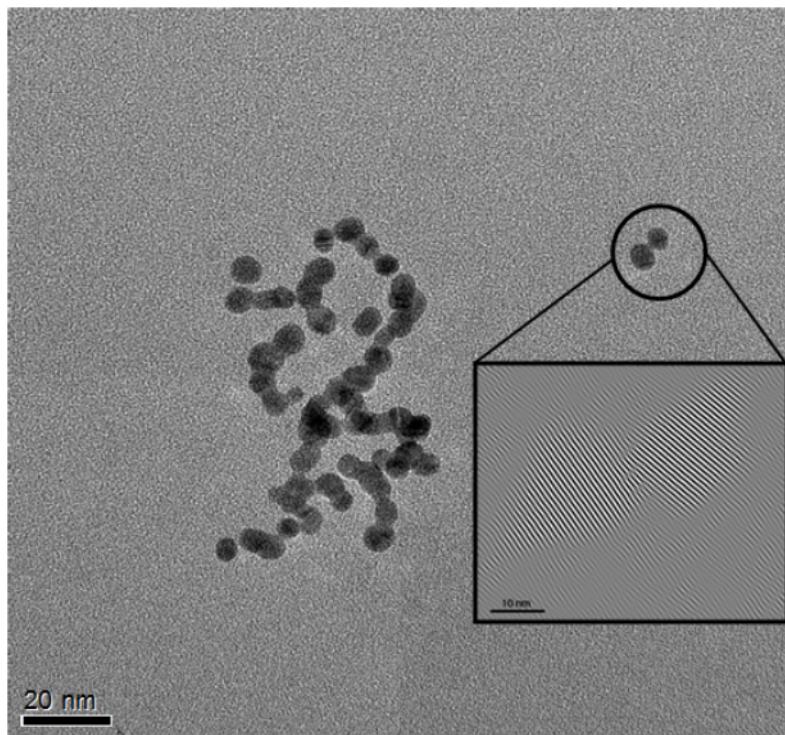
## Small molecule induced one dimensional assembly of Au nanoparticles

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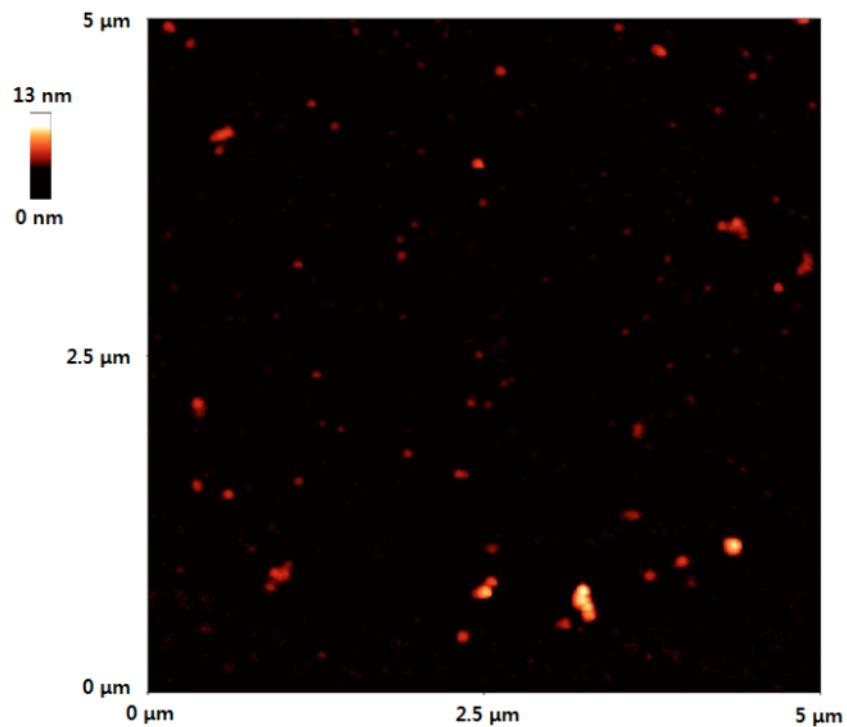
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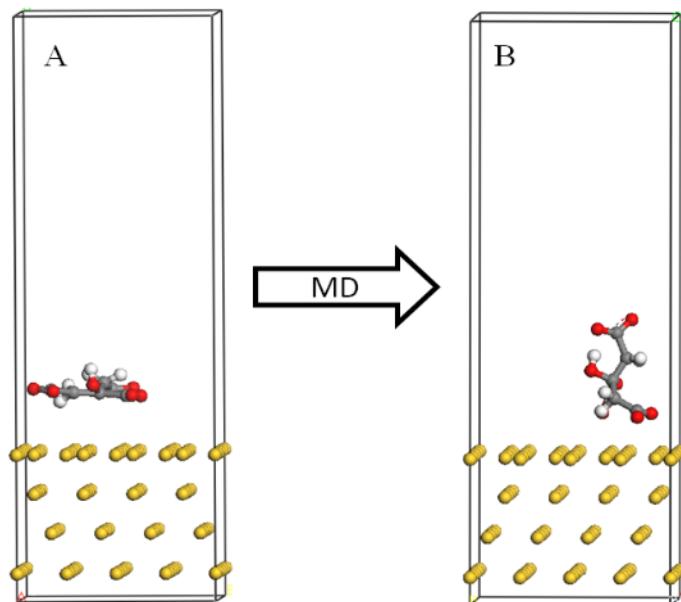
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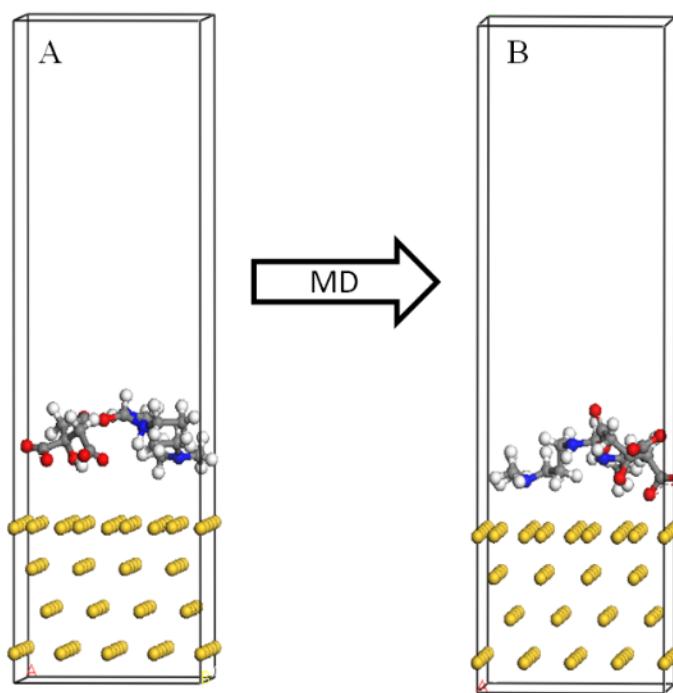
Supplementary Figure (SF) 1: HR-TEM image of Au chains with 0.005 M of EDC and lattice image of Au chains (in a box)



Supplementary Figure (SF) 2: AFM image of Au chains with 0.002M of EDC on the PDDA treated Si wafer (scan rate: 0.3 Hz and scan lines: 512)



Supplementary Figure (SF) 3: snapshots of the Au/Citrate model before and after MD simulation: A. before MD simulation; B. after MD simulation



Supplementary Figure (SF) 4: snapshots of the Au/Citrate-EDC-Citrate model before and after MD simulation: A. before MD simulation; B. after MD simulation

Supplementary Table (ST) 1 non-bonding energies between Au and organism

Surface	Organism	$\square E_{\text{non-bond}}$	$\square E_{\text{vdW}} (\text{kcal}\cdot\text{mol}^{-1})$		$\square E_{\text{coulomb}}$ ( $\text{kcal}\cdot\text{mol}^{-1}$ )
		( $\text{kcal}\cdot\text{mol}^{-1}$ )	Repulsive	Dispersive	
Au (111)	Citrate	$2.214 \times 10^5$	$2.717 \times 10^5$	$-5049 \times 10^4$	-220.121
Au (111)	Citrate-EDC	$2.210 \times 10^5$	$2.719 \times 10^5$	$-5.069 \times 10^5$	-187.793
Au (111)	Citrate-EDC-Citrate	$4.416 \times 10^5$	$5.438 \times 10^5$	$-1.020 \times 10^5$	-178.360