

Supplementary Information Available

**Systematic design and application of unimolecular star-like block copolymer
micelles: a coarse-grained simulation study**

Xiaofang Zhang, Wenjing Lin, Liyang Wen, Na Yao, Shuyu Nie, Lijuan Zhang*

*School of Chemistry and Chemical Engineering, South China University of
Technology, Guangzhou 510640, P R China*

Equilibrium morphology of unimolecular micelles formed from β -CD-*g*-(PLA-*b*-PDMAEMA-*b*-PEtOxMA) aqueous solution is shown in Figure S1 (A), the concentration profile of EtOx beads in three directions (Figure S1 (B)), typical simulated section view (Figure S1 (C)) and density profile (Figure S1 (D)) of the polymeric unimolecular micelle were analyzed from Micell-1 as shown in Figure S1 (A).

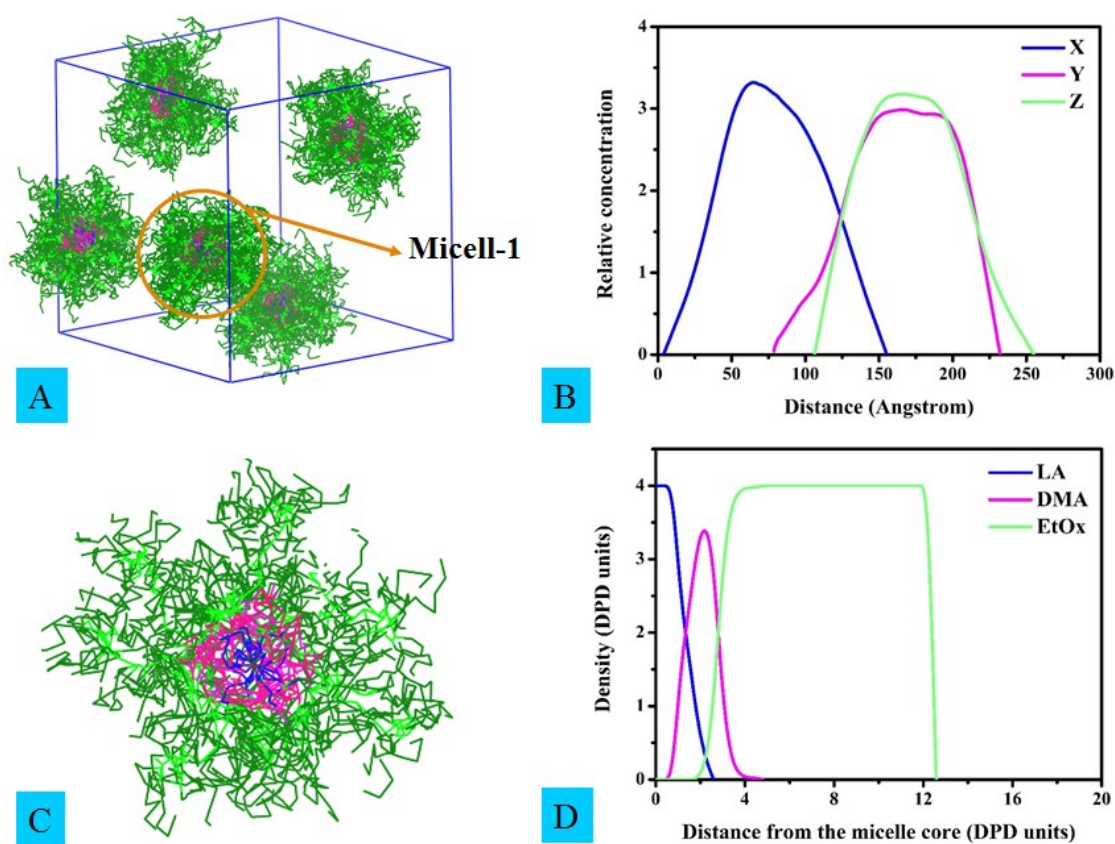


Figure S1. (A) Equilibrium morphologies of unimolecular micelles formed from β -CD-*g*-(PLA-*b*-PDMAEMA-*b*-PEtOxMA) aqueous solution, (B) concentration profile of EtOx beads in three directions, (C) typical simulated section view and (D) density profile of Micell-1.

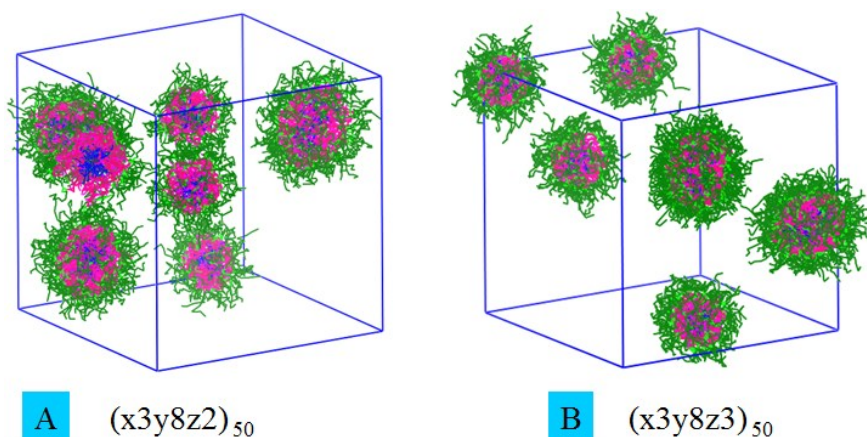


Figure S2. Morphologies of β -CD-*g*-(PLA-*b*-PDMAEMA-*b*-PEtOxMA) micelles of the hydrophilic backbone length z at (A) 2, (B) 3 when polymeric arms number increase to 50.

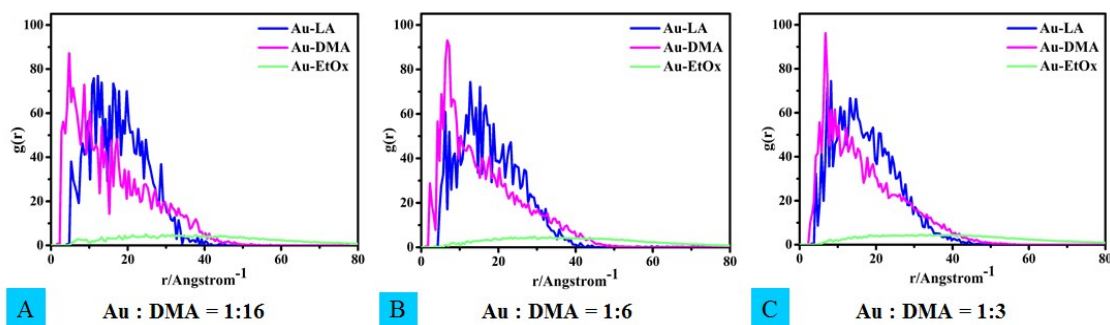


Figure S3. RDF curves of β -CD-*g*-(PLA-*b*-PDMAEMA-*b*-PEtOxMA)/gold nanoparticles at different molar ratios of $[HAuCl_4]:[DMAEMA]$.

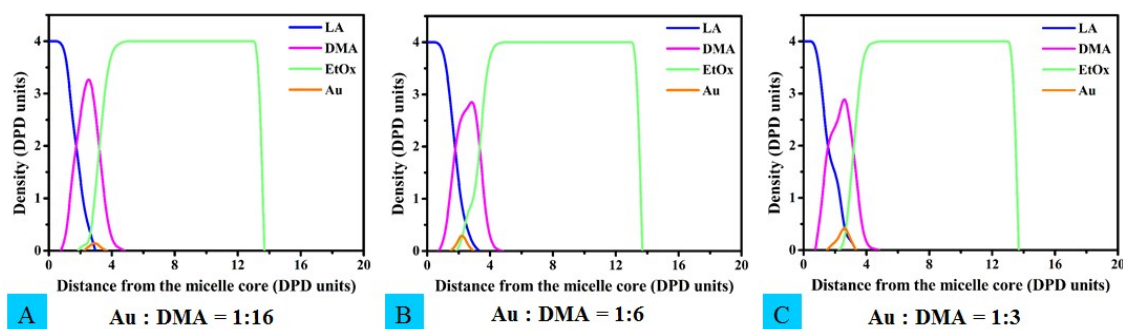


Figure S4. Density profiles of β -CD-*g*-(PLA-*b*-PDMAEMA-*b*-PEtOxMA)/gold nanoparticles at different molar ratios of $[HAuCl_4]:[DMAEMA]$.