

The effect of electric field on the structural order of water molecules around chitosan between nano gold plates by molecular dynamics simulations

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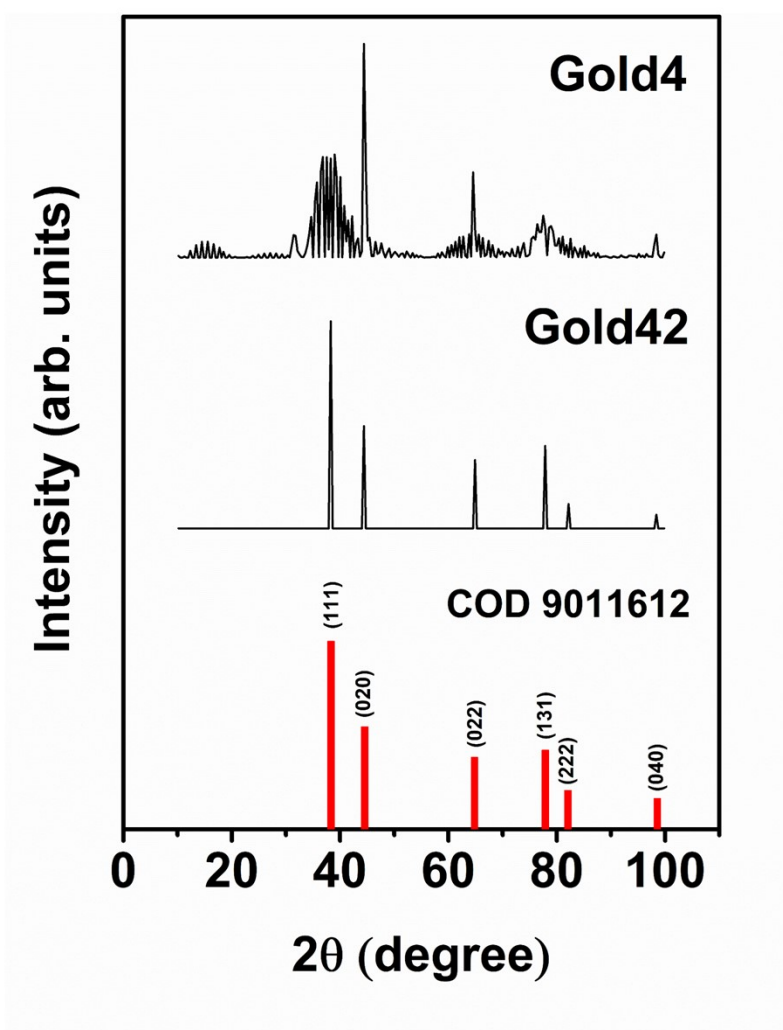


Fig. S1 XRD of gold plates with Gold42 including 42 layers and Gold4 including 4 layers.

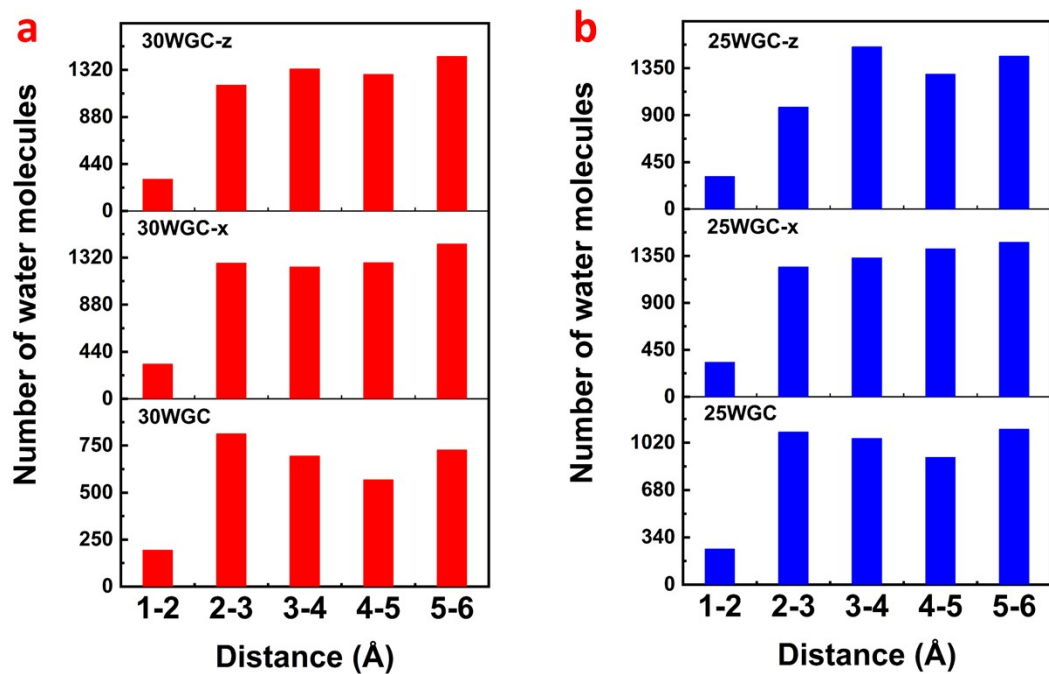


Fig. S2 Number of water molecules around polymers by the shortest distance of oxygen water to chitosan at 300 K and 250 K in systems including WGC, WGC-x, and WGC-z.

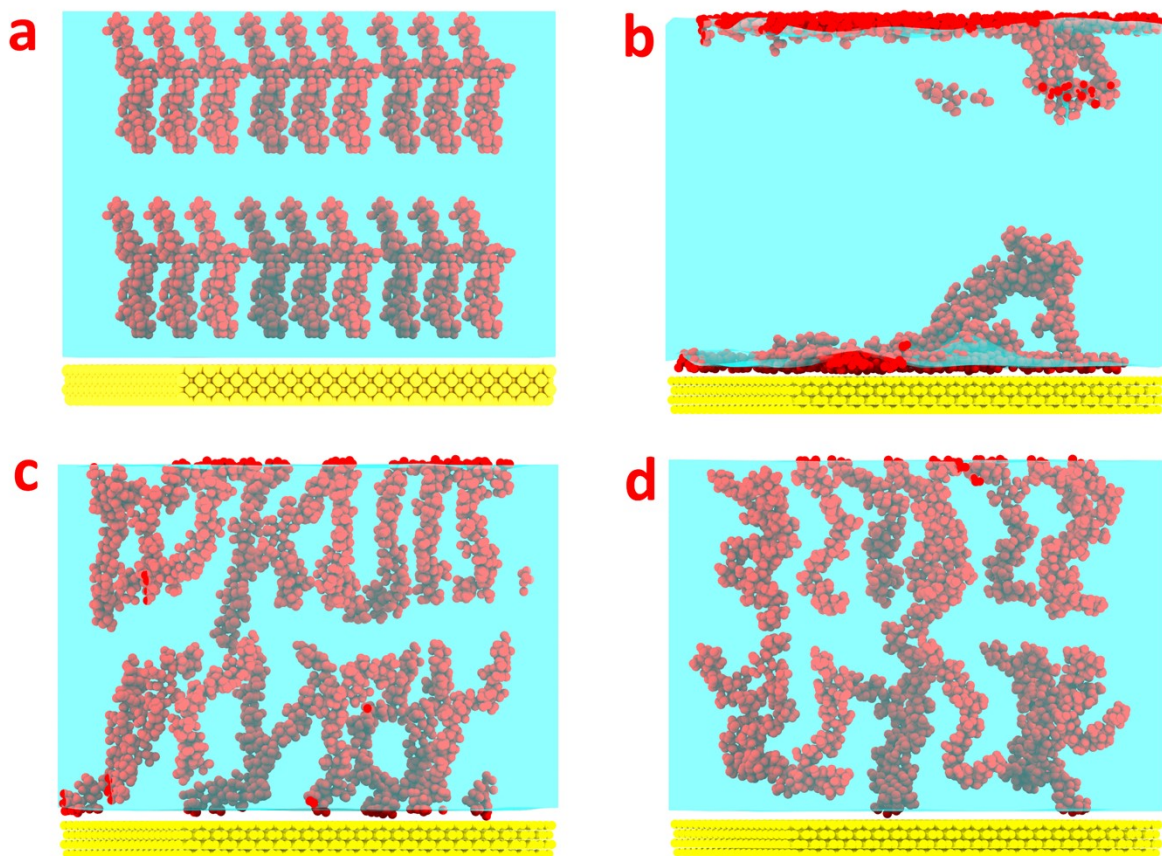


Fig. S3 Snapshots of configurations including 18 chitosan polymers. (a) The initial configurations. (b) The final configurations without the electric field. (c) and (d) The final configurations with the appearing electric field in x- and z-direction, respectively.

Table S1. System specifics of all models.

Name System	Number of polymers	Water molecules	Gold atoms	Temperature	Electric Field
30WG	None	18,225	3,528	300 K	None
30WG-x	None	18,225	3,528	300 K	x-direction
30WG-z	None	18,225	3,528	300 K	z-direction
25WG	None	18,225	3,528	250 K	None
25WG-x	None	18,225	3,528	250 K	x-direction
25WG-z	None	18,225	3,528	250 K	z-direction
30WGC	18	18,225	3,528	300 K	None
30WGC-x	18	18,225	3,528	300 K	x-direction
30WGC-z	18	18,225	3,528	300 K	z-direction
25WGC	18	18,225	3,528	250 K	None
25WGC-x	18	18,225	3,528	250 K	x-direction
25WGC-z	18	18,225	3,528	250 K	z-direction

Table S2. The averaged atomic partial charges of chitosan were calculated from AM1-BCC by Antechamber.

Types of atom	Charge
c	0.7251
c3	0.1432
h1	0.0762
h2	0.0779
hn	0.3631
ho	0.4203
n	-0.4849
n3	-0.9084
o	-0.601
oh	-0.5996
os	-0.4379