Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Structural Order of Water Molecules around the Polyrotaxane including PEG, α-Cyclodextrin, and Linker α -Lipoic acid onto Gold surface by Molecular Dynamics Simulation.

Tue M. N. Le [a], Le Van Sang [b], Hitoshi Washizu*[b]

a Graduate School of Simulation Studies
University of Hyogo
Kobe, Japan
Email: lenhuminhtue@gmail.com

b Graduate School of Information Science
University of Hyogo
Kobe, Japan
Email: h@washizu.org

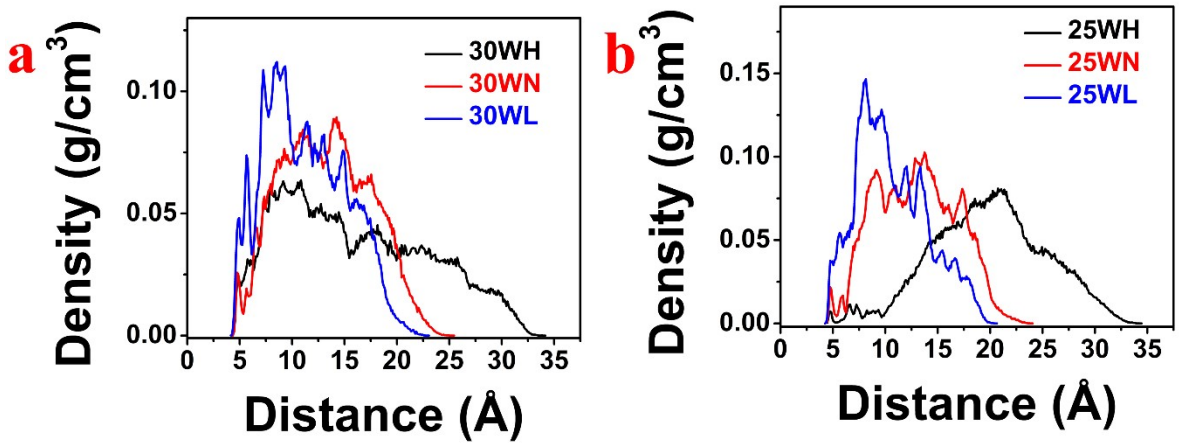
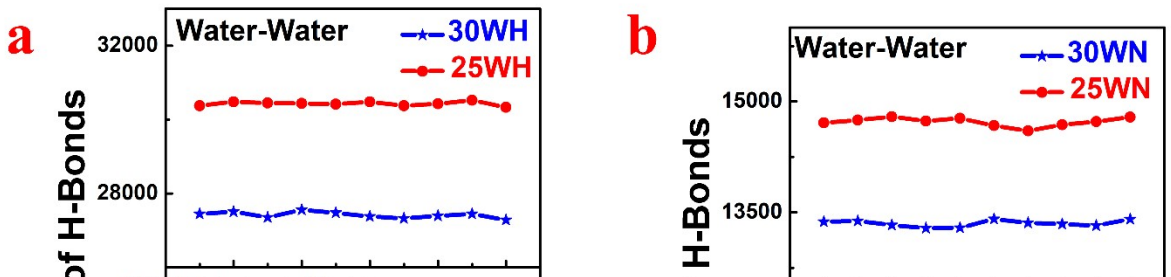


Figure S1. Density of polymer by z-axis at temperatures 300 K and 250 K with models – (a) 30WH, 30WN, 30WL; (b) 25WH, 25WN, 25WL.

Figure S2. Number of H-Bonds at 300 K and 250 K. (a) 30WH and 25WH; (b) 30WN and 25WN; (c) 30WL and 25WL; (d) total average H-bonds of WH, WN, and WL. Water-Water is number H-Bonds between water and water. Polymer-Water is number of H-Bonds between polymer and water.



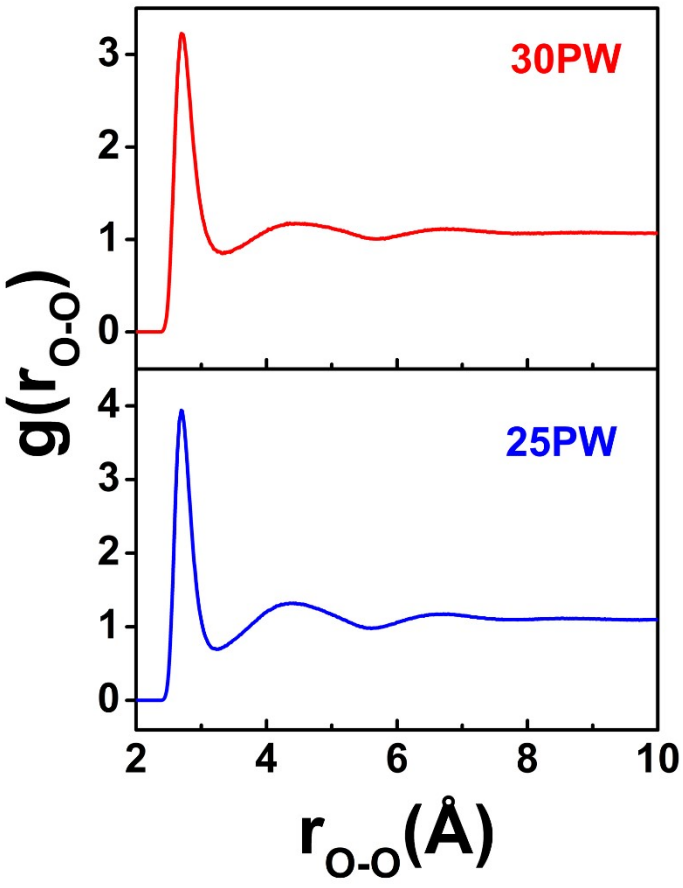


Figure S3. Radial Distribution Function (RDF) of oxygen water in models 30PW and 25PW with 100 frames

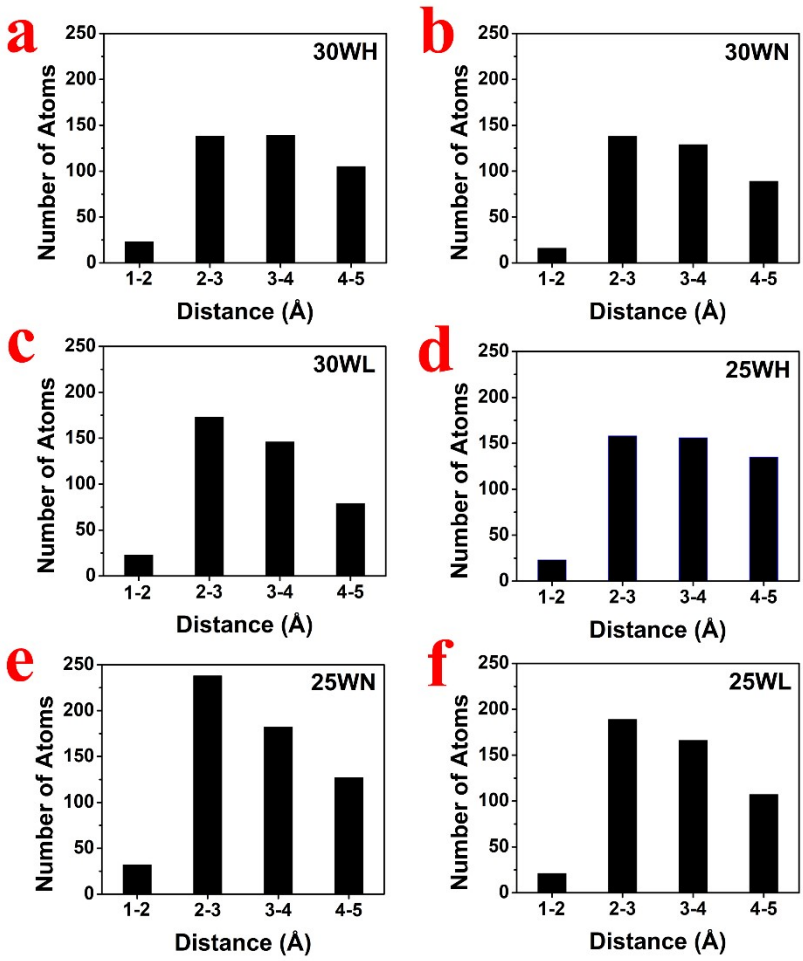


Figure S4. Number of oxygen atoms around polyrotaxane in the last frame at 300 K and 250 K for WH, WN, and WL systems.

Table S1. Total interaction energy (Kcal mol^{-1}) of all atoms: gold-water, gold-polymer, and water-polymer at temperatures 300 K for 30WH, 30WN, 30WL, and 250 K for 25WH, 25WN, 25WL

Models	Gold-Water	Gold-Polymer	Water-Polymer
30WH	-6,045.17	-112.278	-783.734
30WN	-6,204.9	-95.9814	-819.3
30WL	-6,079.66	-169.729	-876.484
25WH	-6,395.27	-24.527	-968.668
25WN	-6,518.28	-86.4425	-1,163.7
25WL	-6,449.24	-159.483	-925.771

Table S2. System specifics of all models

Name Sample	Number of Polymer	Water Molecules	Each plate of gold	Temperature
30WH	1 chain PEG, 3 CDs, 3 Linkers	18,225 molecules	1,764 atoms	300 K
30WN	1 chain PEG, 3 CDs, 3 Linkers	9,025 molecules	1,764 atoms	300 K
30WL	1 chain PEG, 3 CDs, 3 Linkers	4,900 molecules	1,764 atoms	300 K
30WG	none	18,225 molecules	1,764 atoms	300 K
30PW	none	18,225 molecules	none	300 K
25WH	1 chain PEG, 3 CDs, 3 Linkers	18,225 molecules	1,764 atoms	250 K
25WN	1 chain PEG, 3 CDs, 3 Linkers	9,025 molecules	1,764 atoms	250 K
25WL	1 chain PEG, 3 CDs, 3 Linkers	4,900 molecules	1,764 atoms	250 K
25WG	none	18,225 molecules	1,764 atoms	250 K
25PW	none	18,225 molecules	none	250 K

Table S3. Averaged charges of atoms. The α-CD and ALA linker were taken from density functional theory calculations using the B3LYP/6-31G(d,p) by Gaussian software. For PEG, the atomic partial charges were calculated from AM1-BCC by Antechamber.

CD+linker

Type atom	Charge
c3	0.165558
h1	0.045993
h2	0.099463
hc	0.041664
ho	0.409587
oh	-0.6091
os	-0.49723
ss	-0.13224
c	0.721409
o	-0.52741

PEG

Type atom	Charge
c3	0.126092
h1	0.043854
ho	0.4015
oh	-0.6028
os	-0.42826