Supplementary Material

for

Porous organic cage as an inhibitor of $A\beta_{42}$ peptide: a simulation study

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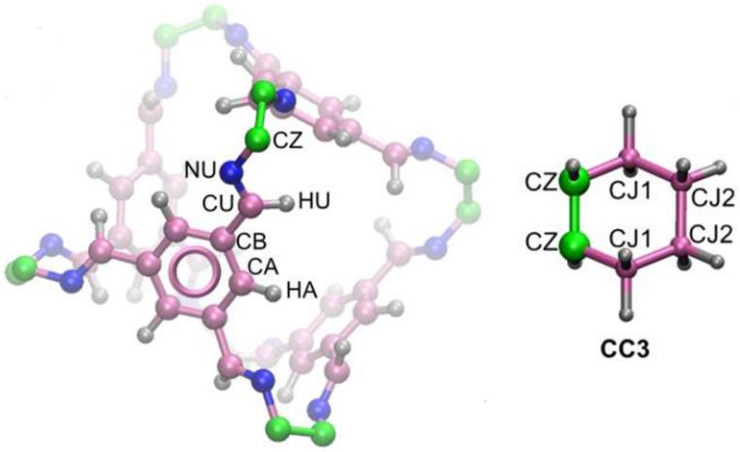

Figure S1. Atom types in CC3[1, 2].

Table S1. Non-bonded parameters in CC3[1, 2].

Atom type	σ (nm)	ε (kJ/mol)	Charge(e)
CA	0.355	0.2929	0.00
HA	0.242	0.1255	0.06
CB	0.355	0.2929	-0.16
CU	0.350	0.3347	0.47
HU	0.250	0.2092	0.00
NU	0.325	0.7113	-0.62
CZ	0.350	0.2761	0.22
HZ	0.250	0.1255	0.03
CJ1	0.350	0.2761	-0.13
HJ1	0.250	0.1255	0.05
CJ2	0.350	0.2761	0.07
HJ2	0.250	0.1255	-0.02

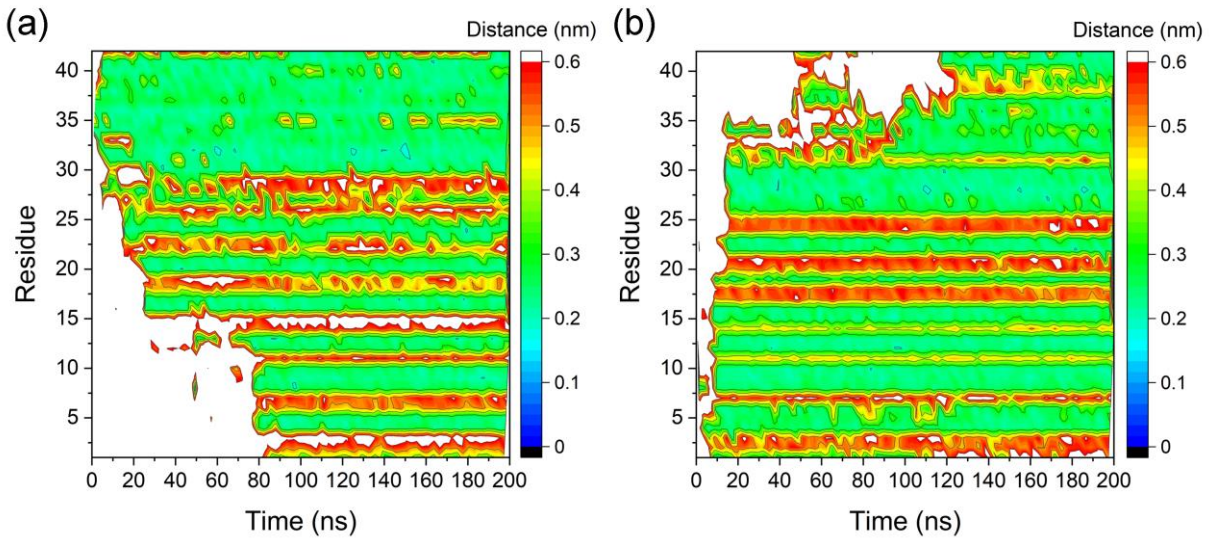

Figure S2. The residue contact maps of $A\beta_{42}$ peptide adsorbed on CC3 surfaces (a) plane and (b) sphere.

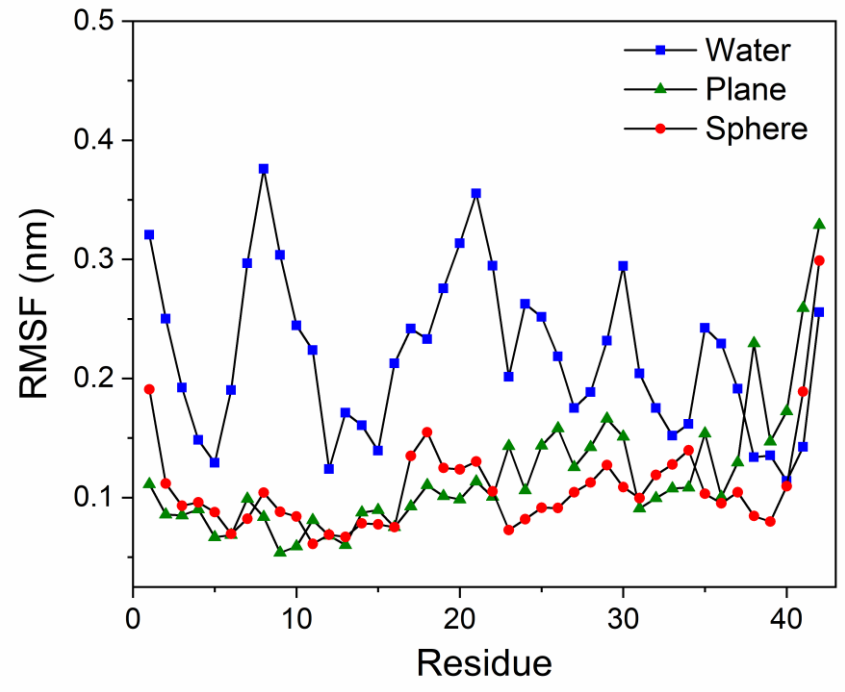

Figure S3. RMSF of C_α atoms of $A\beta_{42}$ peptide averaged over the last 40 ns trajectory.

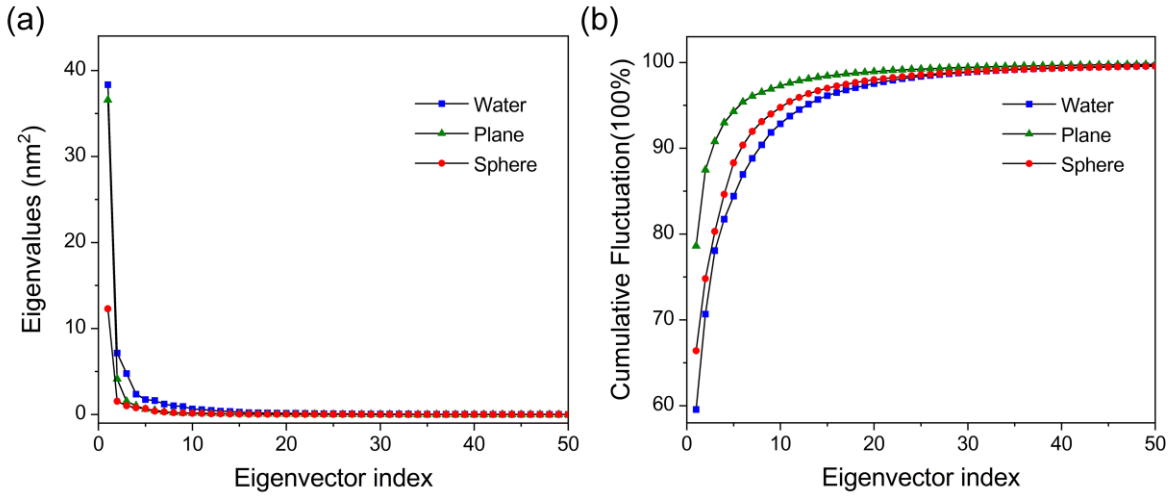

Figure S4. The (a) eigenvalues (nm^2) and (b) cumulative percentages (%) of the first 50 eigenvectors derived from PCA analysis of the Aβ_{42} peptide backbone atoms in water and on the CC3 crystals versus eigenvector indices.

References

1. M. J. Bojdys, T. Hasell, N. Severin, K. E. Jelfs, J. P. Rabe and A. I. Cooper, *Chem. Commun.*, 2012, **48**, 11948-11950.

2. X. Kong and J. Jiang, *Phys. Chem. Chem. Phys.*, 2017, **19**, 18178-18185.