

Supporting Information

Insights into the Oil Adsorption and Cyclodextrin Extraction Process on Rough Silica Surface by Molecular Dynamics Simulation

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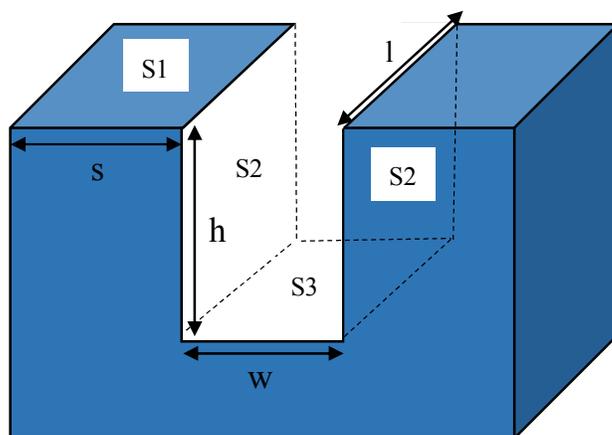


Fig. S1 Side view of the unit structure of the silica groove with width (w), height (h), step width (s), and length (l).

Table S1 Force field parameters for dodecane, silica and β -cyclodextrin in this study

Species	Atom type	Non-bond parameters		
		charge	Sigma (nm)	Epsilon(kJ/mol)
Silica	Tetrahedral silicon	2.100	0.37064	7.70065×10^{-6}
	Bridging oxygen	-1.050	0.35532	0.6495
	Hydroxyl oxygen	-0.950	0.35532	0.6495
	Hydroxyl hydrogen	0.425	0	0
Dodecane	Carbon in CH ₃ group	-0.270	0.36527	0.32635
	Carbon in CH ₂ group	-0.180	0.35814	0.23430
	Carbon in CH ₁ group	-0.090	0.35636	0.13389
	Hydrogen in CH ₃ group	0.090	0.23876	0.10042
	Hydrogen in CH ₂ group	0.090	0.23876	0.14644
	Hydrogen in CH ₁ group	0.090	0.23876	0.18828
β -cyclodextrin	Carbon in the ring connected with OH	0.140	0.35636	0.13389
	Carbon in the ring	0.100	0.35636	0.13389
	Carbon in the ring connected with another	0.300	0.35636	0.13389
	Carbon in the chains	0.050	0.35814	0.23430
	Oxygen in the ring	-0.400	0.29399	0.41840
	Oxygen in the OH group	-0.660	0.31538	0.63639
	Hydrogen in the chains	0.090	0.04000	0.19246
	Hydrogen in the rings	0.100	0.04000	0.19246
	Hydrogen in the OH group	0.430	0.04000	0.19246
Bonds for clayFF force field				
Species i	Species j	b_0 (nm)	k_b (kJ/mol/nm ²)	
Hydroxyl oxygen	Hydroxyl hydrogen	0.1	463532.808	

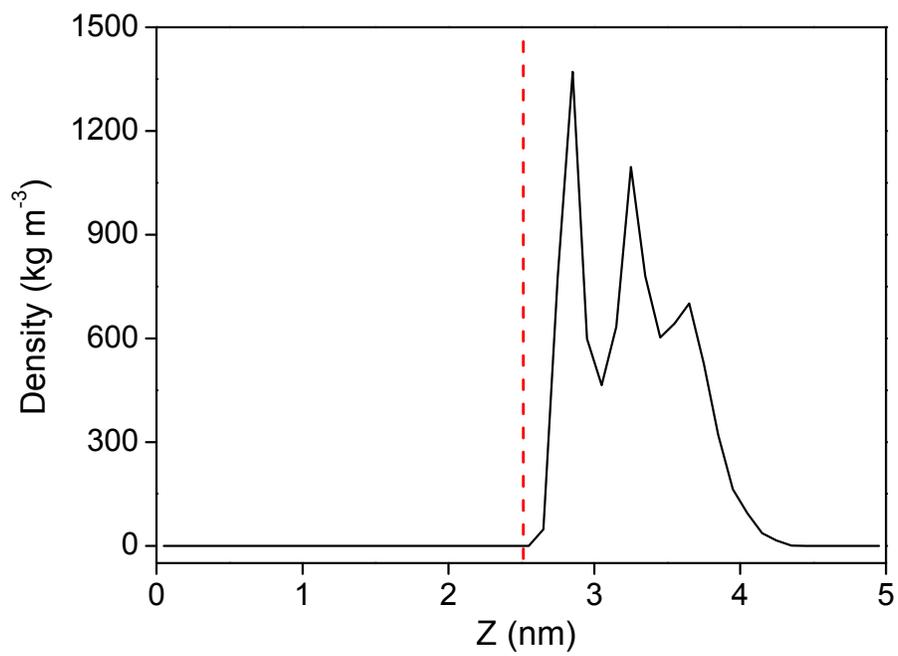


Fig. S2 Density profile of oil along the z-direction on the smooth silica surface. Red dotted line represents the top of the silica surface.

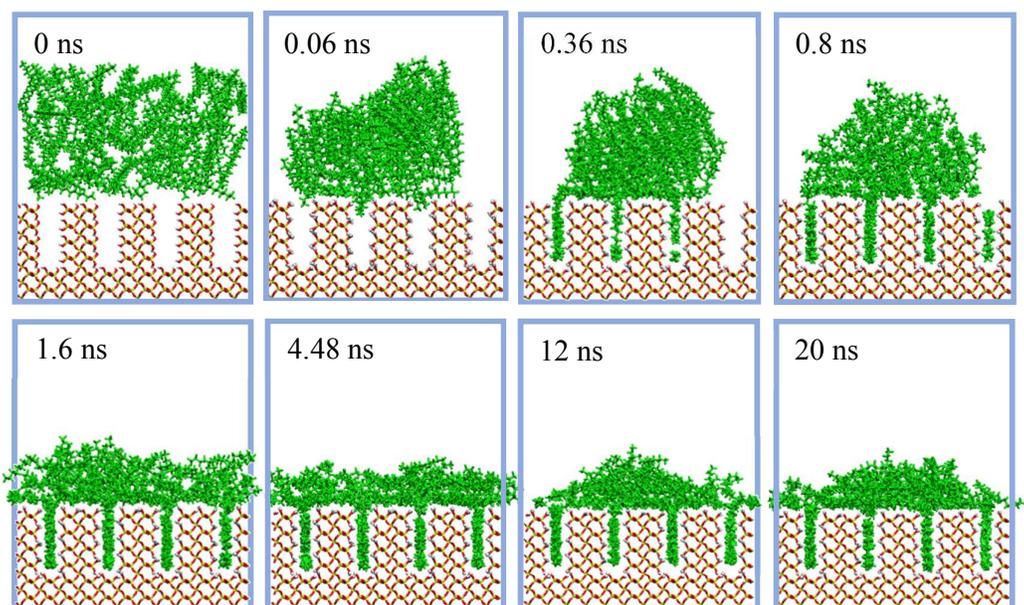


Fig. S3 Snapshots of oil (green) during adsorption on the rough silica surface (R₄)

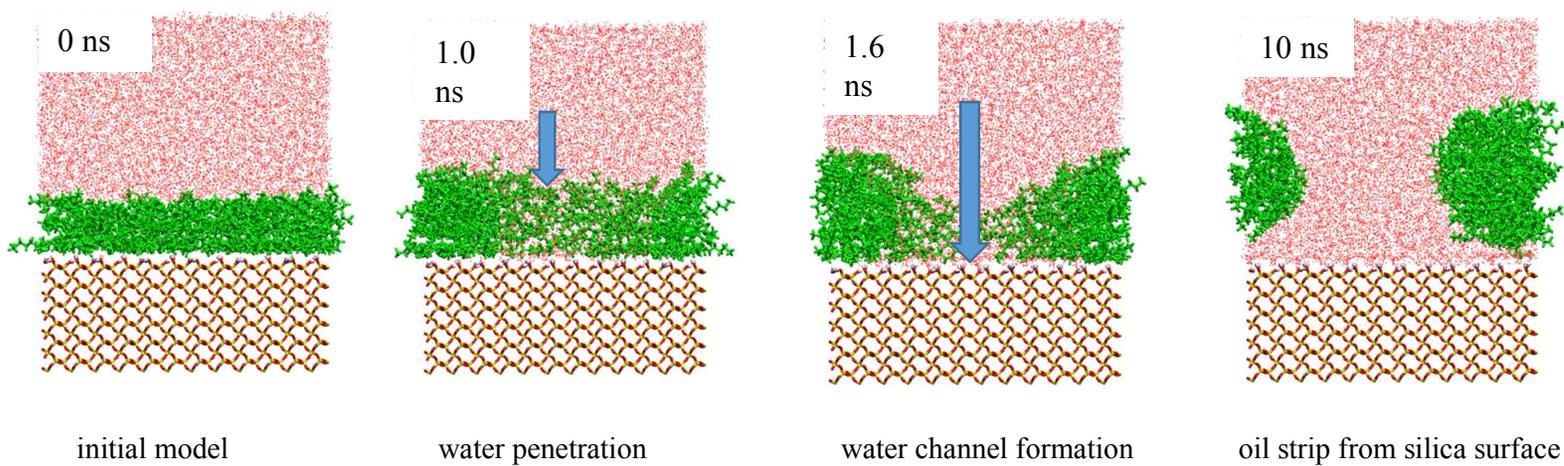


Fig. S4 Snapshots of the oil (green) detachment process from the smooth silica surface (R_0) in water (red)

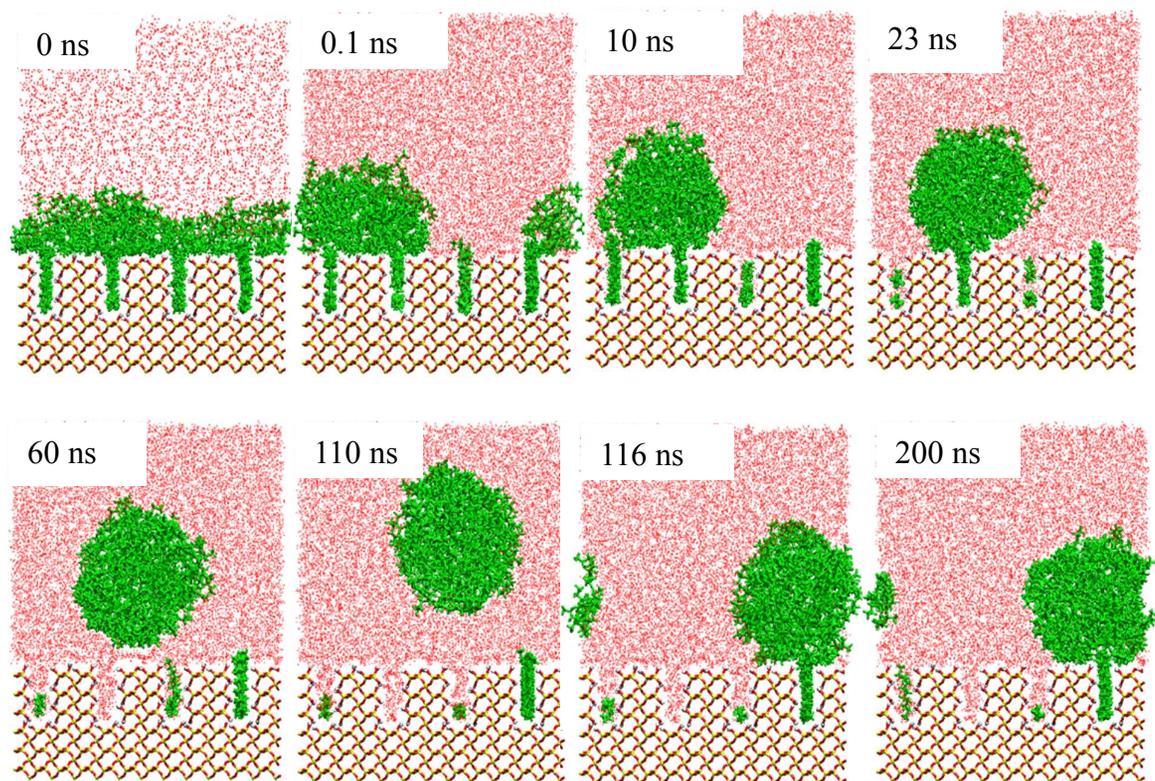


Fig. S5 Snapshots of oil droplet (green) movement above the silica surface (R₃) in water (red)

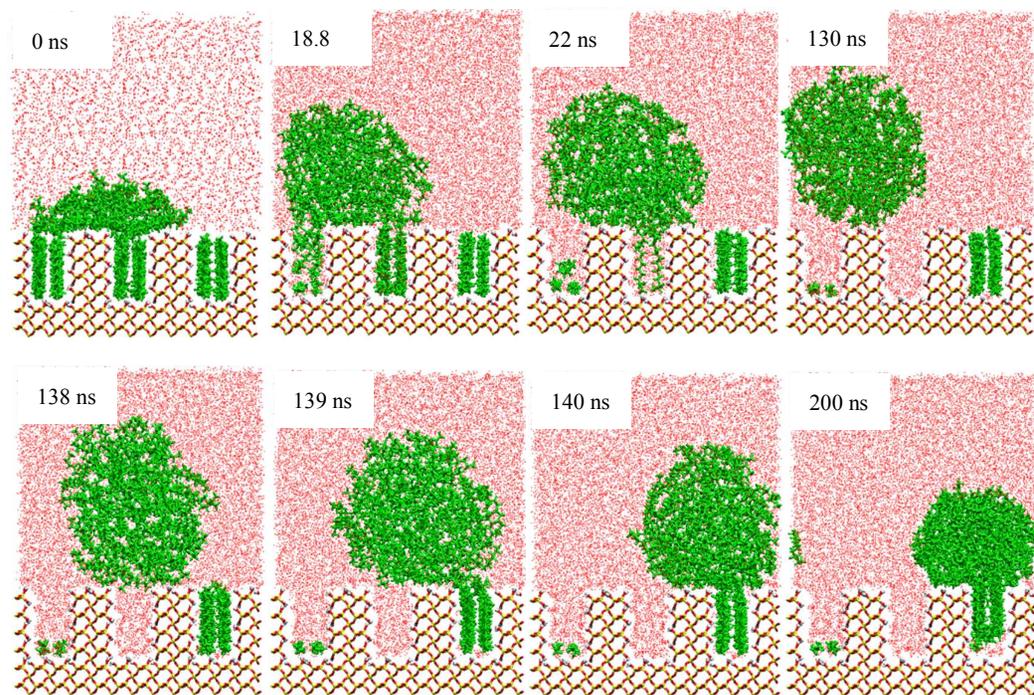


Fig. S6 Snapshots of oil droplet (green) movement above the silica surface (R₂) in water (red).

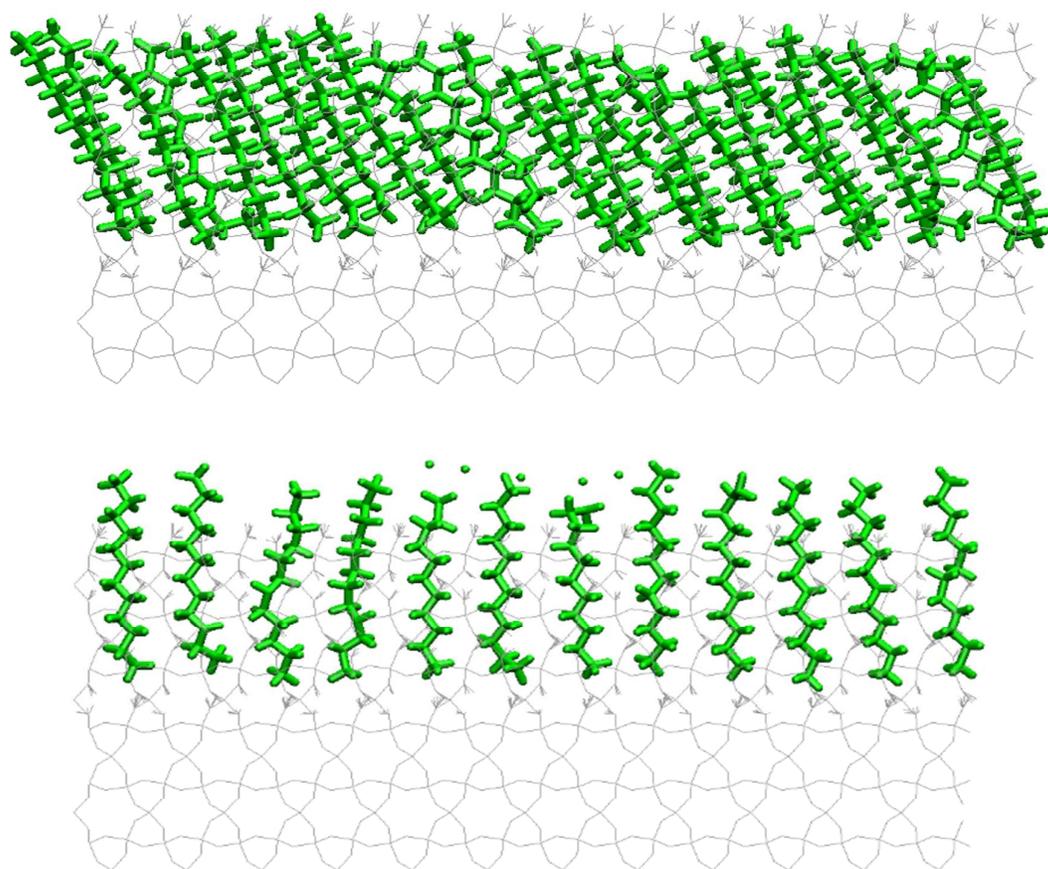
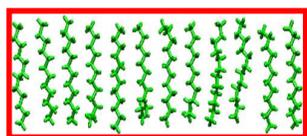
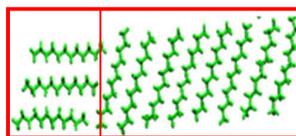


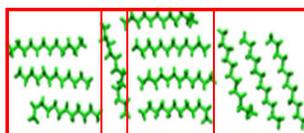
Fig. S7 Molecular configuration of the residual oil molecules inside the silica groove (top: surface R₂; bottom: surface R₃)



A



B



C

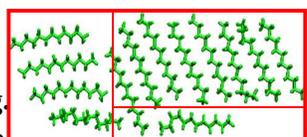


Fig. Configuration of oil clusters inside the groove. Panel A shows only one cluster because all oil molecules are parallel to each other. Panel B shows two clusters which contains 3 and 8 oil molecules, respectively. Panel C shows three clusters which contains 1, 4 and 8 oil molecules, respectively. Panel D shows four clusters which contains 3, 1, 4, and 3 oil molecules, respectively.

D

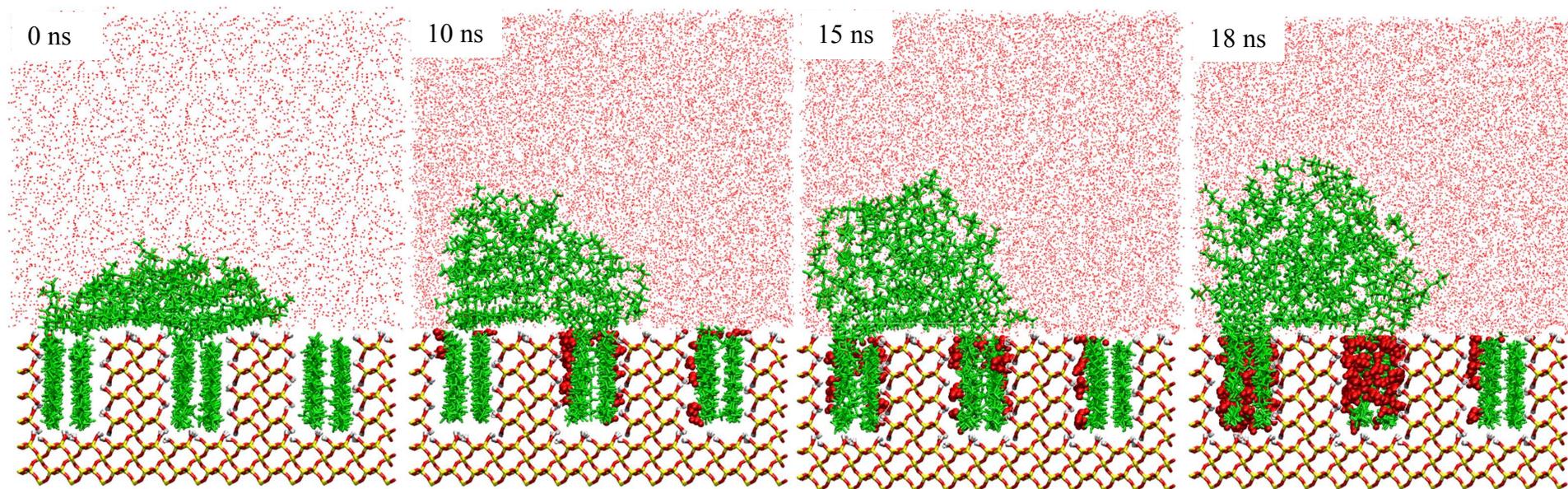


Fig. S9 Penetration of water (red) through the interfaces between the sequestered oil (green) and the internal well of silica grooves (R_2).