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

Supporting Information

The Influence of Silica Nanoparticle Geometry on the Interfacial Interactions of Organic Molecules: A Molecular Dynamics Study

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Table S1. Force field parameters for silica surface[1] and phthalic acid molecule

SILICA NANOPARTICLE

Atoms	σ (nm)	ε (kJ × mol^{-1})	Charge (e)
Si (bulk)	0.33855	2.44704	0
Si (surface)	0.33855	2.44704	+0.31
O (bulk)	0.29	0.58576	0
O (silanol)	0.312	0.71128	-0.71
O^- (silanol deprotonated)	0.312	0.71128	-1.31
H (silanol)	0	0	+0.4
Na^+	0.333045	0.011598	+1.0
Bonds	**b_0 (nm)**	**k_b (kJ × mol^{-1} × nm^{-2})**	
Si-O	0.163	251040	
O-H	0.0945	462750.4	
Angle	**θ_0 (deg)**	**k_θ (kJ × mol^{-1} × rad^{-2})**	
Si-O-Si	155	397.48	
O-Si-O	109.5	397.48	
Si-O-H	109.5	397.48	

PTHALIC ACID MOLECULE

Atoms	σ (nm)	ε (kJ × mol^{-1})	Charge (e)
CA (aromatic)	0.355	0.292880	-0.115
HA (aromatic)	0.242	0.125520	0.115
CAC (aromatic carbon of carboxylate)	0.355	0.292880	-0.115
C (carboxylate)	0.355	0.292880	0.635
H (carboxylate)	0	0	0.450
O (carboxylate, C-OH)	0.312	0.711280	-0.530
O (carboxylate, C-O)	0.296	0.878640	-0.440
Bonds	**b_0 (nm)**	**k_b (kJ × mol^{-1} × nm^{-2})**	
CA-CA	0.140	392460	
CA-HA	0.108	307110	
CA-C	0.149	334720	
C-OH	0.136	376560	
C-O	0.123	476980	
O-H	0.0945	462750	
Angle	**θ_0 (deg)**	**k_θ (kJ × mol^{-1} × rad^{-2})**	
CA-CA-CA	120	527.18	
CA-CA-HA	120	292.88	
CA - CA - C	120	711.28	
CA - C - OH	120	585.76	
CA - C - O	120.4	669.44	
C - O - OH	113	292.88	
OH - C - O	121	669.44	

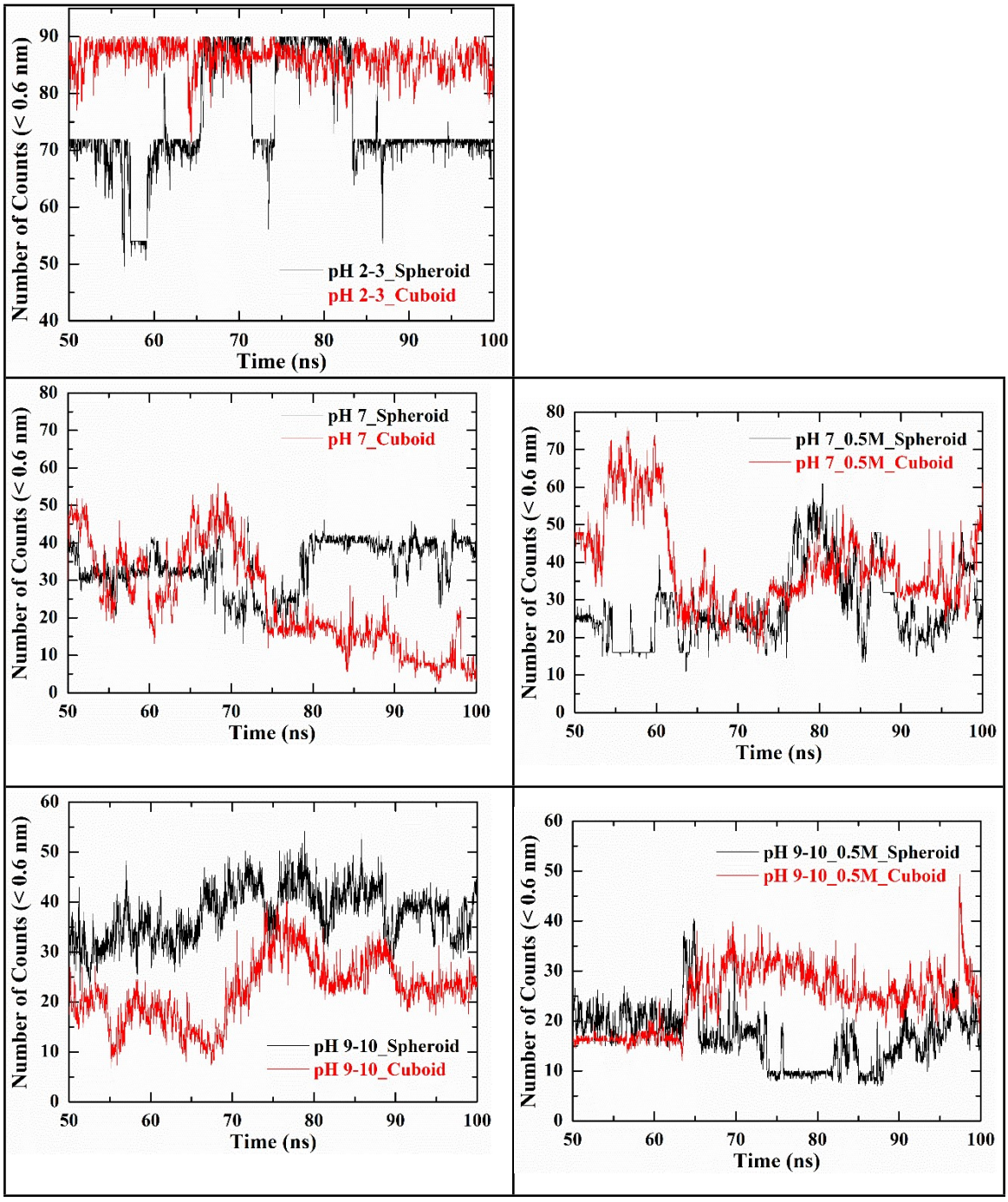

Figure S1. Plots representing the number of counts for the minimum distance of approach of PHTHA molecules towards the geometries of silica nanoparticle at various pH conditions.

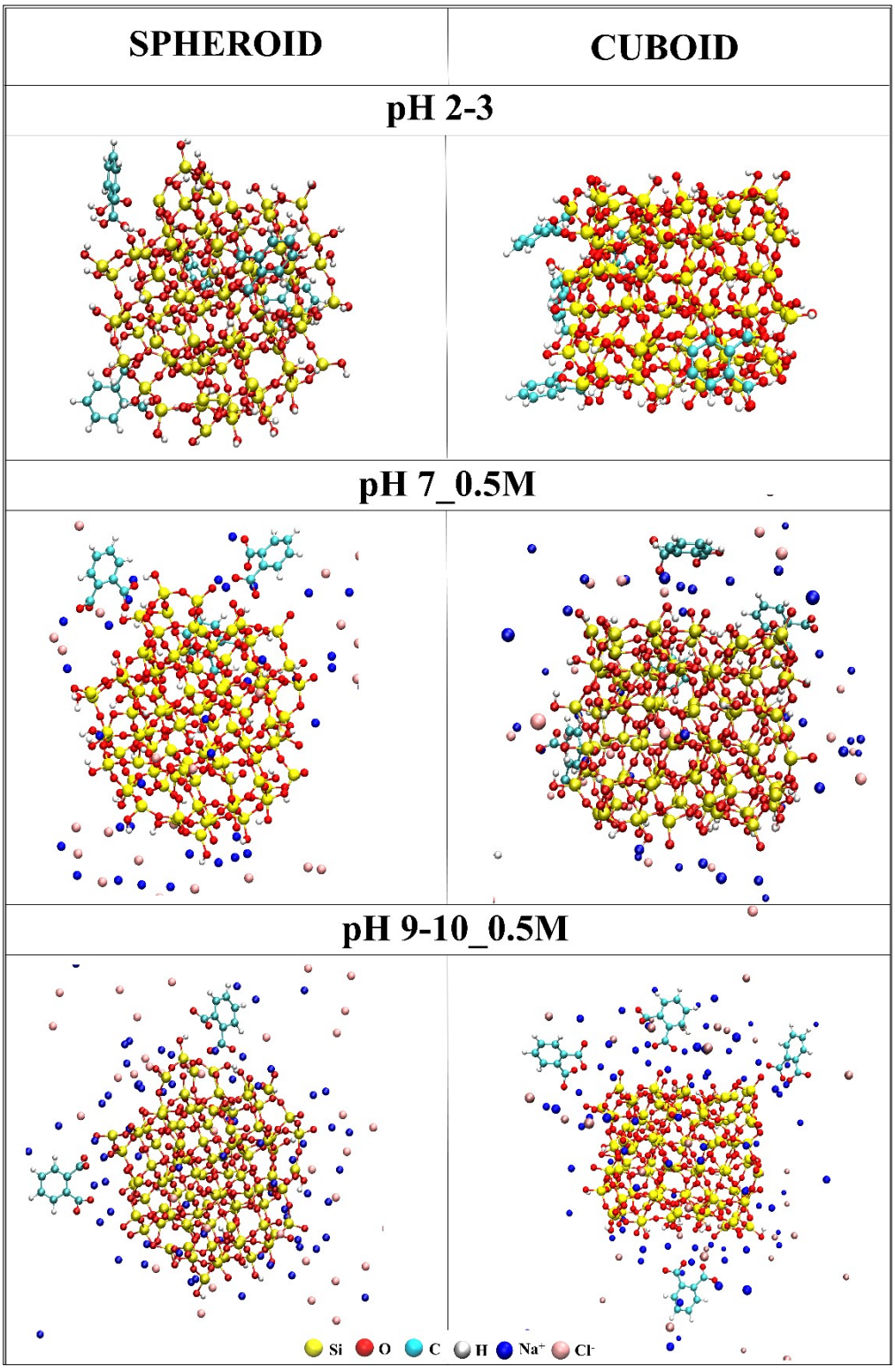

Figure S2. Snapshots from the trajectories of MD simulation representing the binding structure and orientation of PHTHA molecules towards the spheroid and cuboid geometries of silica nanoparticle at various pH conditions of aquatic environment.

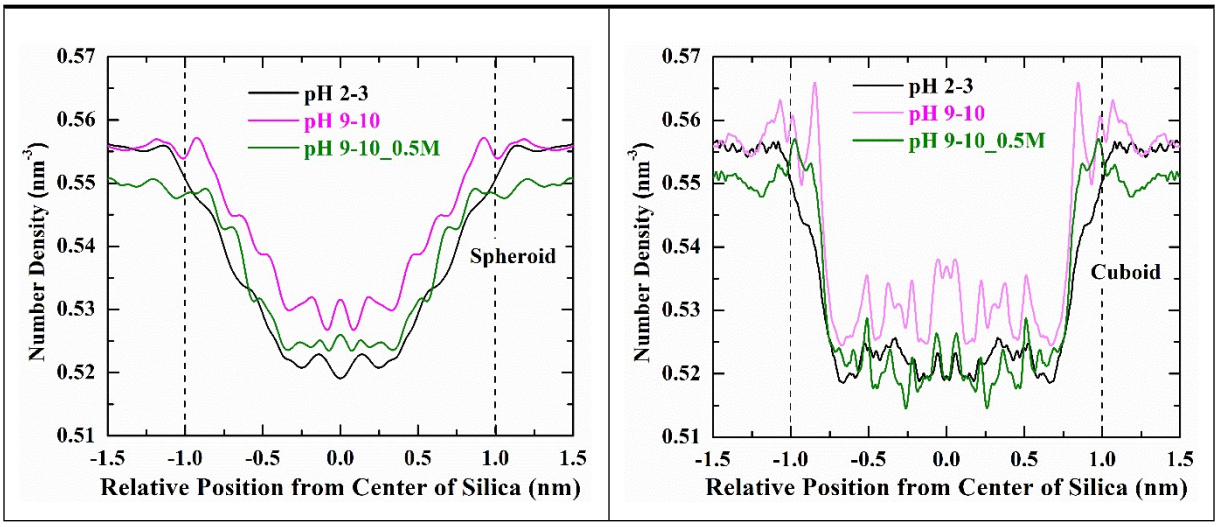

Figure S3. Number density of water molecules at the silica geometry interface; (a) Spheroid; (b) Cuboid; dotted lines represent the interface of silica nanoparticle geometry.

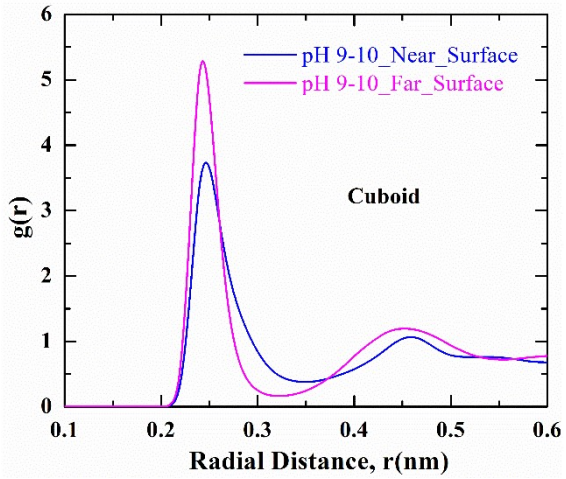

Figure S4. Co-ordination of water molecules around the Na^+ ions of cuboid geometry.

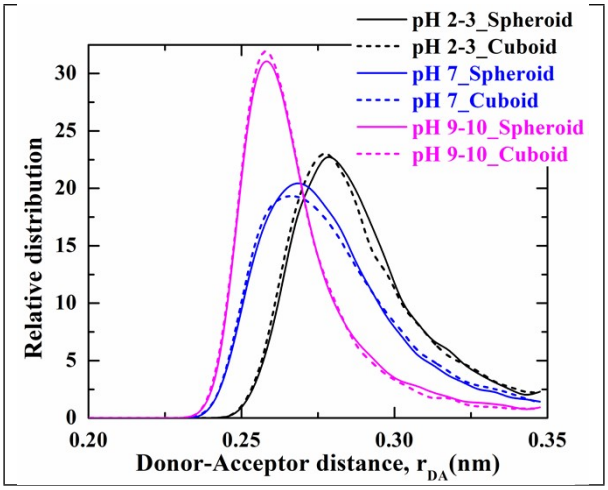

Figure S5. Donor-Acceptor distance for the hydrogen bonds formed at the silica-water interface.

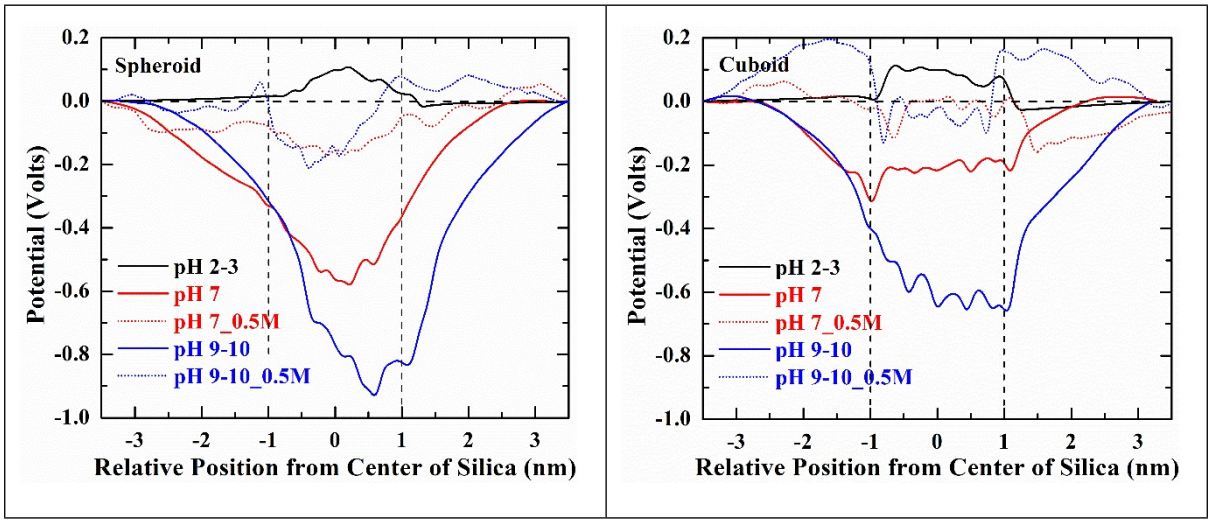

Figure S6. Electrostatic potential profiles for spheroid and cuboid geometry of silica nanoparticles at various pH conditions; dotted lines represent the silica nanoparticle geometry.

References

1 K. Kolman and Z. Abbas, Molecular dynamics exploration for the adsorption of benzoic acid derivatives on charged silica surfaces, *Colloids Surfaces A*, 2019, **578**, 123635.