

Electronic Supplementary Information

RGD tripeptide onto perfect and grooved rutile surfaces in aqueous solution: adsorption behaviors and dynamics

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Fig. S1

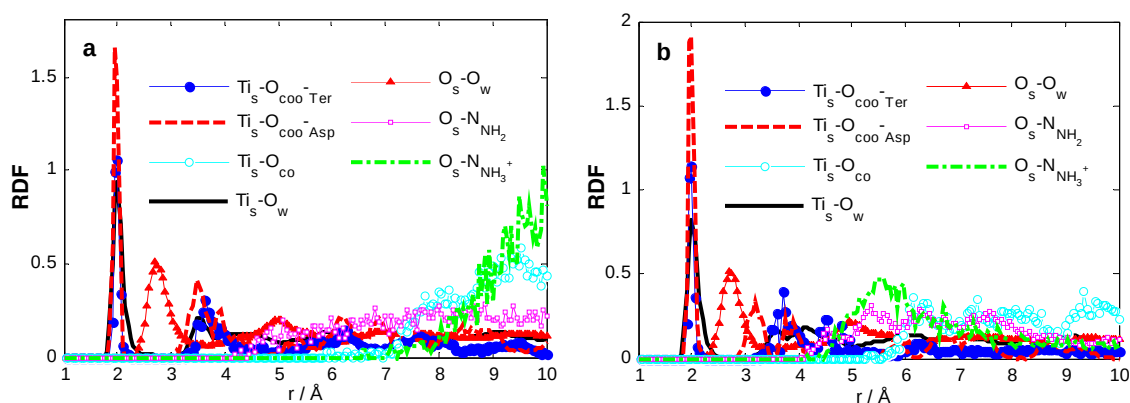


Fig. S1 RDFs of TiO₂ surface-water, RGD for model III and model IV. (a) Model III. (b) Model IV.

Fig. S2

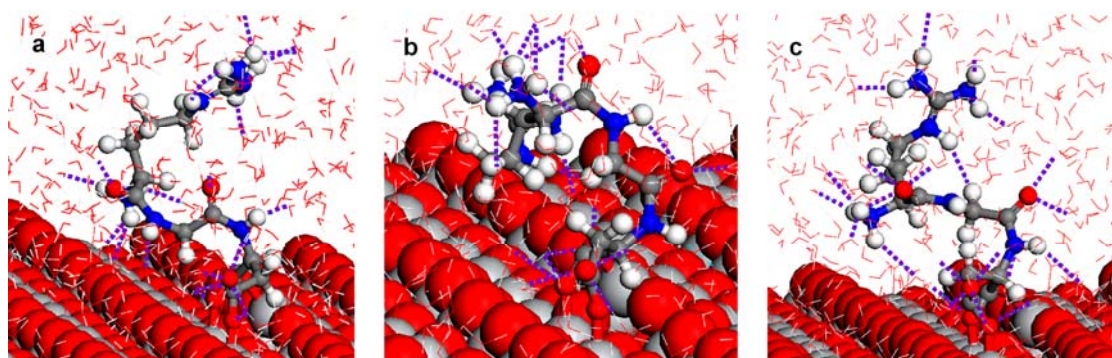


Fig. S2 Adsorption conformations of RGD onto perfect TiO₂ surface. (a) 300 ps. (b) 600 ps. (c) 900 ps. TiO₂, RGD and water molecules are shown by CPK mode, ball-and-stick mode and line mode, respectively. Hydrogen bonds between RGD and water are represented by purple dotted lines.

Fig. S3

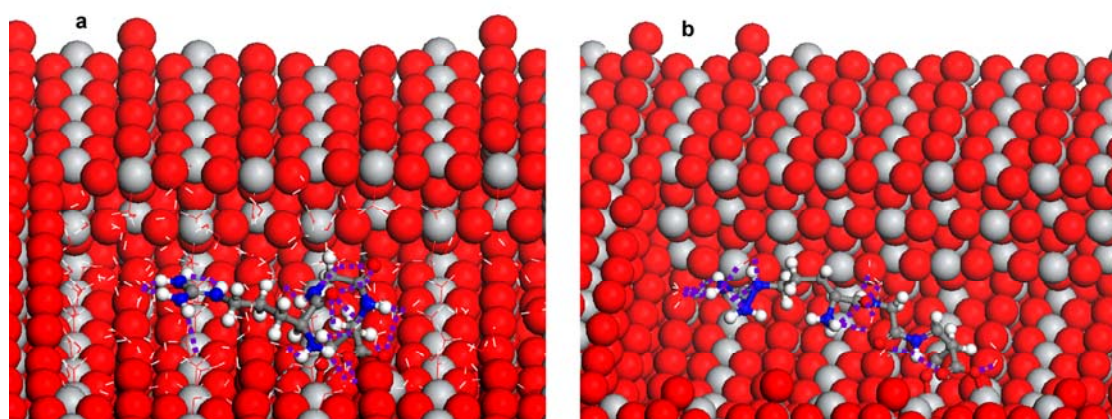


Fig. S3 Adsorption conformations of RGD onto groove ii and groove iii TiO₂ surfaces. (a) Groove ii at 600 ps, only water molecules in the interior of groove ii are visualized. (b) Groove iii at 900 ps, only water molecules forming hydrogen bonds with RGD are visualized. TiO₂, RGD and water molecules are shown by CPK mode, ball-and-stick mode and line mode, respectively. Hydrogen bonds between RGD and water are represented by purple dotted lines.

Fig. S4

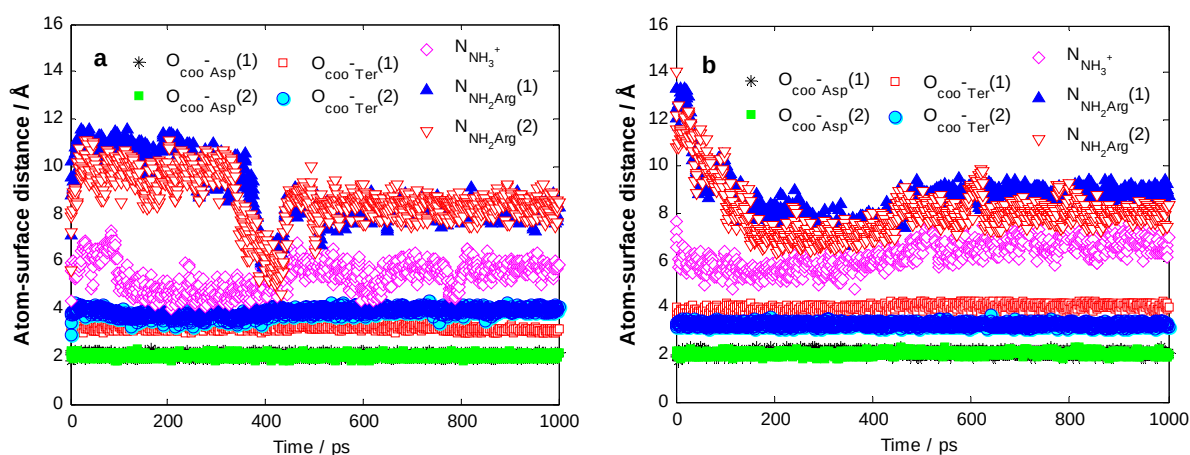


Fig. S4 Evolutions of RGD atom-surface distances for model III and IV during the molecular dynamics simulation time. (a) Model III. (b) Model IV.

Fig. S5

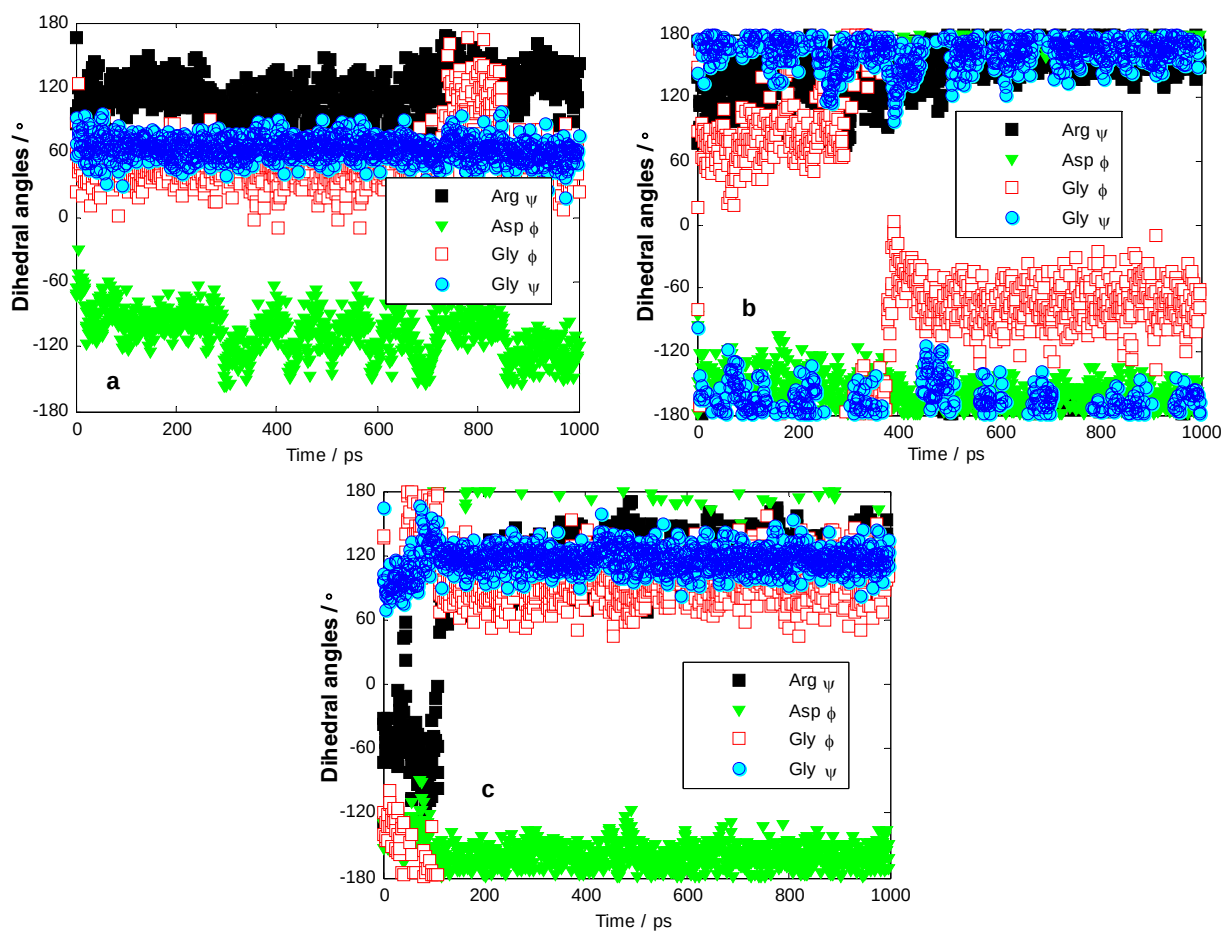


Fig. S5 Evolutions of backbone dihedral angles of RGD adsorbed onto rutile TiO_2 (110) grooved surfaces during the molecular dynamics simulation time. (a) Model II. (b) Model III. (c) Model IV.

Fig. S6

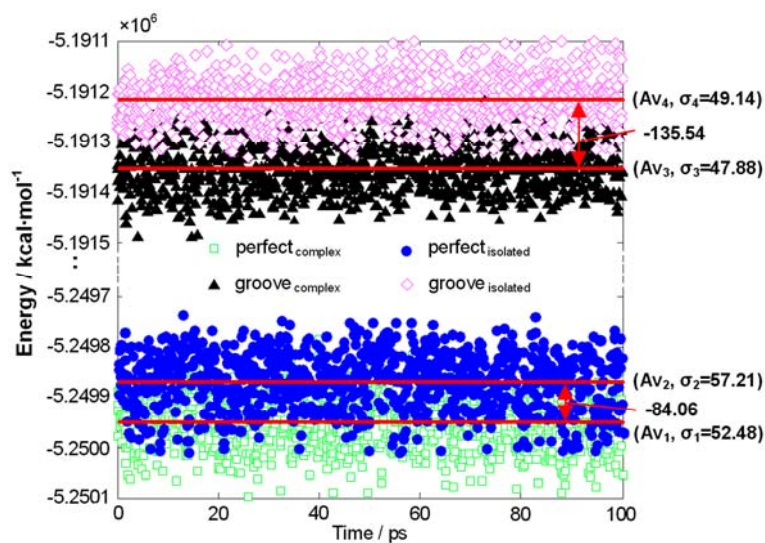


Fig. S6 Energy distributions for both equilibrating interacting and noninteracting systems of perfect and groove i models during the last 100ps MD equilibration stage. Average values (Av) for the corresponding systems are shown by red lines ($Av_1=-5249953.41$ kcal·mol⁻¹, $Av_2=-5249869.35$ kcal·mol⁻¹, $Av_3=-5191354.08$ kcal·mol⁻¹, $Av_4=-5191218.54$ kcal·mol⁻¹).

Fig. S7

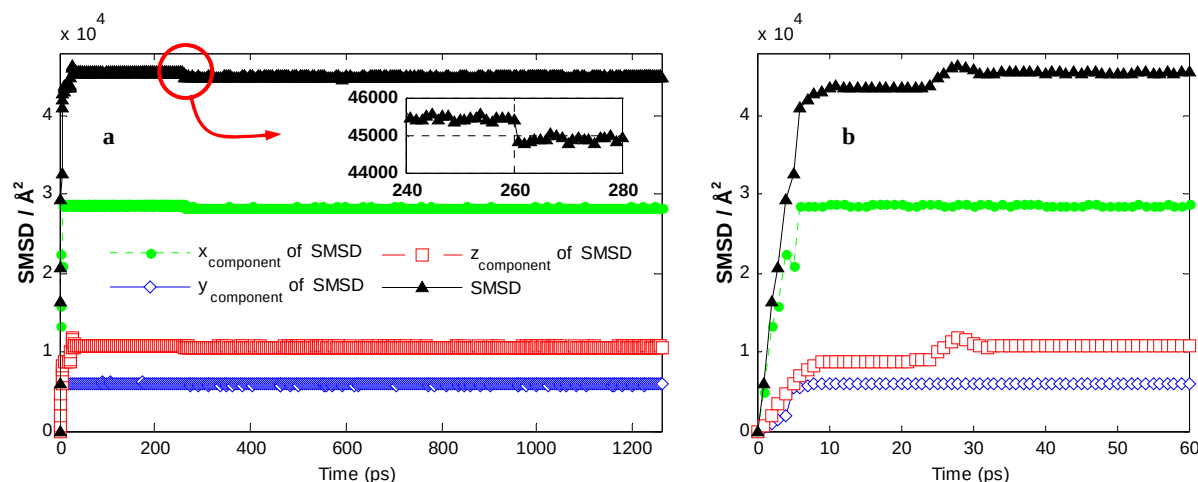


Fig. S7 SMSD for all water molecules in the first hydration layer above the perfect surface during molecular dynamics simulation time. (a) SMSD during the whole simulation stage after energy minimization. (b) SMSD during the first 60ps after energy minimization.

Table S1

Table S1 Statistical parameters of atom-surface distances / Å

atom	model I		model II		model III		model IV	
	mean	σ	mean	σ	mean	σ	mean	σ
O _{coo} -Asp(1)	3.81	0.22	2.00	0.08	2.06	0.07	2.09	0.08
O _{coo} -Asp(2)	2.08	0.08	2.05	0.08	2.02	0.08	2.05	0.08
O _{coo} -Ter(1)	2.17	0.10	3.77	0.21	3.21	0.11	3.98	0.15
O _{coo} -Ter(2)	3.25	0.12	4.22	0.59	3.87	0.17	3.09	0.09
N _{NH₃⁺}	6.74	1.09	5.67	0.78	5.38	0.62	6.23	0.66
N _{NH₂} -Arg(1)	9.63	2.33	9.58	1.34	8.86	1.30	8.66	1.07
N _{NH₂} -Arg(2)	9.14	1.86	9.67	1.40	8.90	1.06	8.03	1.14