Electronic Supplementary Material (ESI) for Biomaterials Science
This journal is © The Royal Society of Chemistry 2013

Molecular dynamics study on pH response of protein adsorbed on peptide-modified polyvinyl alcohol hydrogel

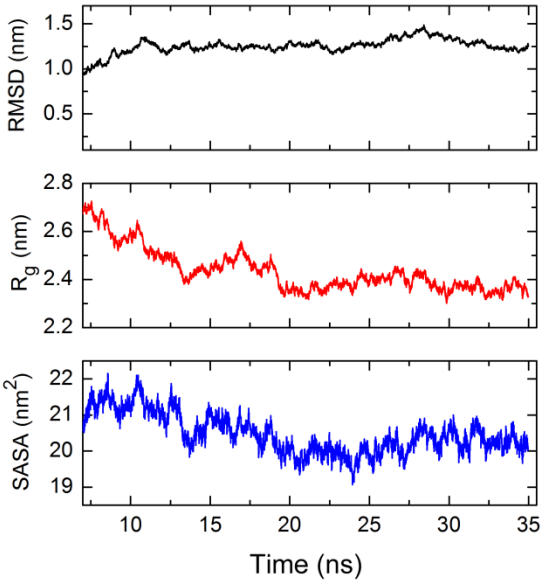
Supporting Information

Table S1. Summary of residues to be protonated at pH 3.0

Chain	Residue	Index	pKa	Chain	Residue	Index	pKa
L	ASP	17	3.3	H	ASP	62	3.9
		82	3.7			73	3.2
		151	3.8			102	4.0
						151	3.0
	GLU	81	3.4		GLU	108	3.6
		105	4.4			215	3.3
		123	3.6				
		143	4.6			1	3.9
		161	5.4			6	5.1
		165	3.0			46	4.2
		187	3.5			89	4.6
		195	3.7			155	4.6
		213	4.6			219	3.5
Ligand	ASP	270	3.9				
	GLU	269	3.3				

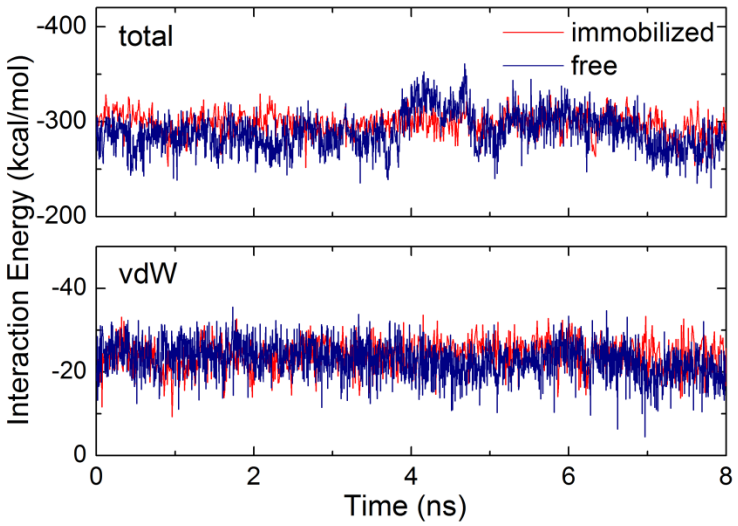
This journal is © The Royal Society of Chemistry 2013

Fig. S1. The root mean square deviations (RMSD) (first row) of carbon atoms in PVA, radius of gyration (Rg) (second row) and solvent accessible surface area (SASA) (third row) of PVA in prolonged simulation of protein-hydrogel system at pH 3.0 .



This journal is © The Royal Society of Chemistry 2013

Fig. S2 Interaction energies of protein-free SBL ligand (blue) and protein-immobilized SBL ligand (red) at pH 7.0



This journal is © The Royal Society of Chemistry 2013

Fig. S3 a b) Conformational changes of protein and SBL after immobilization at pH 7.0;. c,d) Conformational changes of PVA matrix after alignment by protein backbone at different pH. Free system without PVA is shown in Green; system at pH 7.0 is shown in blue; system at pH 3.0 is shown in magenta. Proteins are displayed by NewCartoon model; PVA chains are displayed by Licorice model; SBL is displayed by VDW model. Proteins are shown in transparent for clarity in(c, d).