Supplementary Material for

Molecular Simulation of Fibronectin Adsorption onto Polyurethane Surfaces

Melisa Panos[†], Taner Z. Sen[‡] and M. Göktuğ Ahunbay[*,†]

[†] Department of Chemical Engineering, Istanbul Technical University, Istanbul, Turkey.

[‡] U.S. Department of Agriculture – Agricultural Research Service, Corn Insects and Crop Genetics Research Unit and Dept. of Genetics, Development and Cell Biology, Iowa State University, Ames, IA.

*Corresponding author: ahunbaym@itu.edu.tr

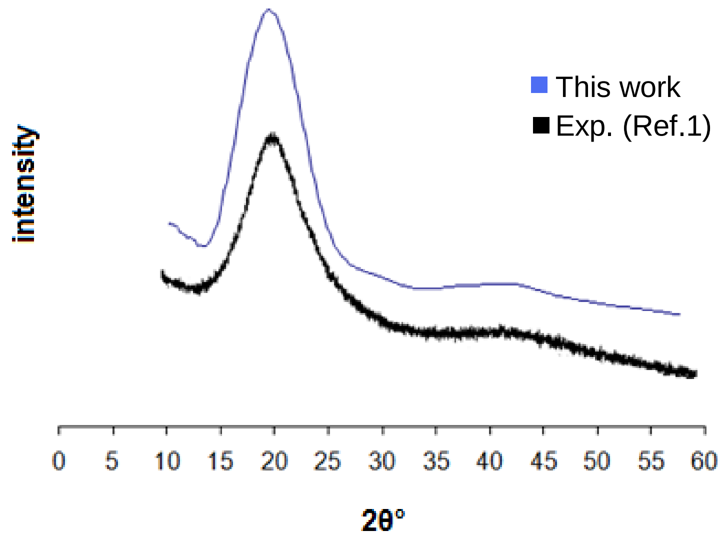

Figure S1. Experimental [1] and simulated x-ray pattern of amorphous CO-HDI polymer

Table S1. Structural and mechanical properties of amorphous PVA and CO-HDI

Property	**Method**	**PVA**	**CO-HDI**
Young modulus	This work	5.43	1.76
(GPa)	Experimental [2]	4.34+/-0.017	
Poisson ratio	This work	0.31	0.37
	Experimental [3]	0.426-0.447	
Radius of gyration	This work	8.17	16.61
(Å)	Experimental [4]	11.4	
Cohesive energy density	This work	138.87	
(cal/cm3)	Experimental [4]	158-201	
Solubility parameter	This work	11.78	
$(cal/cm^3)^{1/2}$	Experimental [4]	12.6-14.2	

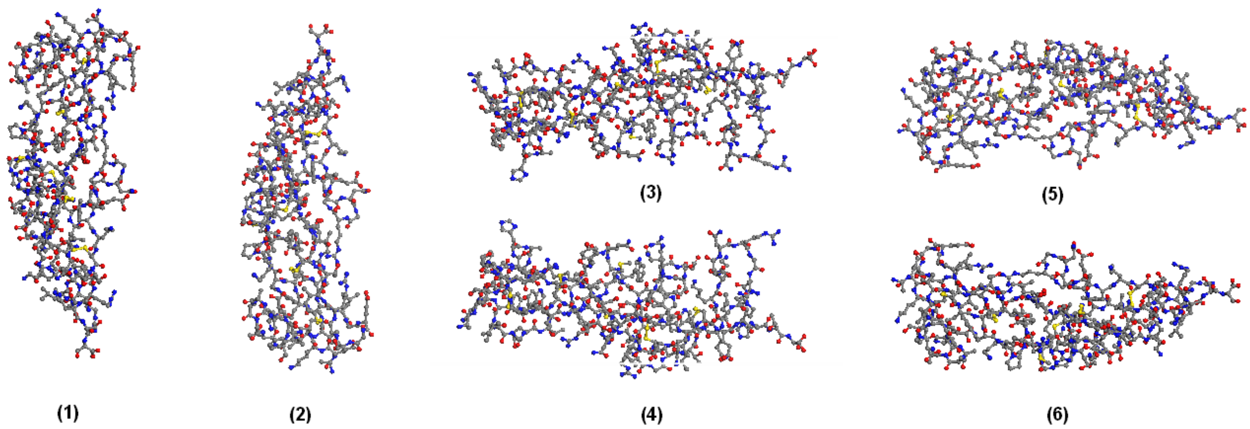

Figure S2 : Fibronectin domain 1FBR in six different initial orientations perpendicular to the polymer surfaces. Hydrogen atoms are omitted for the purpose of clarity.

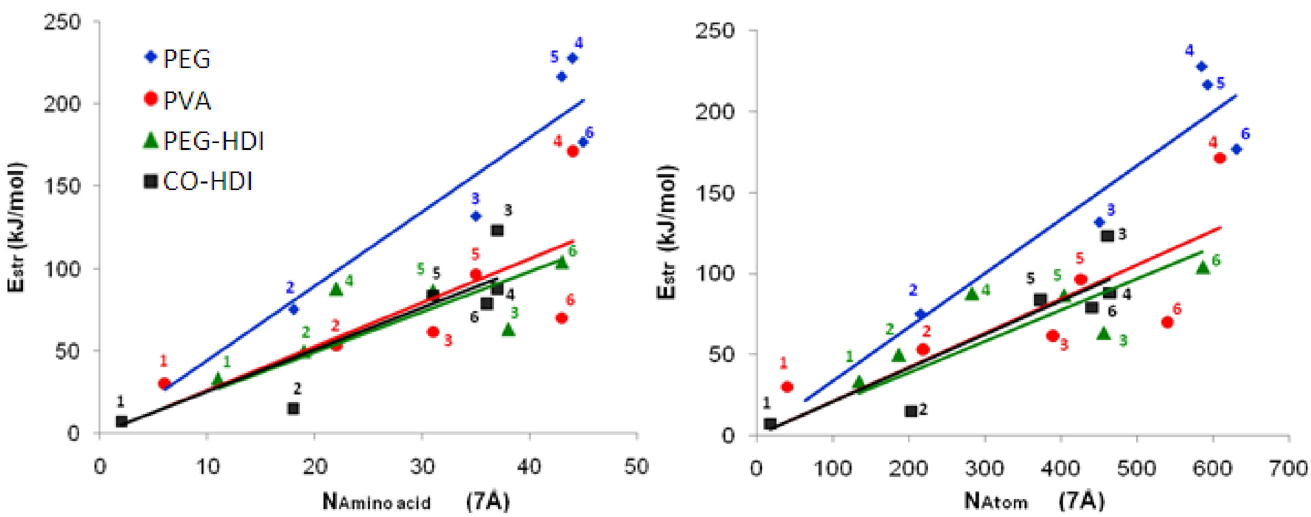

Figure S3. Strain energies with respect to protein amino acids and atoms within an adsorption layer of δ = 7Å on the polymer surface after energy minimization. Numbers next to the data marks indicate the initial orientation of the protein above the surface as defined in Figure S2.

Table S3. Absolute protein-surface interaction energies E_{int} (kJ/mol) and strain energies E_{strain} (kJ/mol) after energy minimization as function of the adsorption layer thickness (δ) based on the number of amino acids (N_{AA}) and on the number of protein atoms (N_{Atom}).

		N_{AA}			N_{Atom}		
E_{int} (kJ/mol)		**δ = 3 Å**	**δ = 5 Å**	**δ = 7 Å**	**δ = 3 Å**	**δ = 5 Å**	**δ = 7 Å**
	PEG	25.01	19.66	15.16	5.67	1.70	1.12
	PVA	19.73	13.32	10.25	4.84	1.39	0.81
	PEG-HDI	28.23	20.10	15.30	6.20	1.94	1.20
	CO-HDI	23.93	15.68	11.88	5.93	1.60	0.97
E_{strain} (kJ/mol)		**δ = 3 Å**	**δ = 5 Å**	**δ = 7 Å**	**δ = 3 Å**	**δ = 5 Å**	**δ = 7 Å**
	PEG	7.49	5.84	4.49	1.67	0.51	0.33
	PVA	5.04	3.50	2.65	1.29	0.37	0.21
	PEG-HDI	4.80	3.29	2.46	1.01	0.32	0.19
	CO-HDI	4.52	3.38	2.54	1.29	0.35	0.21

Table S4. Number of amino acids (N_{AA}) adsorbed on the polymer surfaces in the most favorable orientation for δ = 7Å after energy minimization.

PEG-HDI Orientation 6	**N_{AA}**	**CO-HDI Orientation 3**	**N_{AA}**	**PEG Orientation 5**	**N_{AA}**	**PVA Orientation 4**	**N_{AA}**
GLY	4	GLY	4	ARG	5	THR	6
SER	4	CYS	3	ASN	4	GLY	4
ASP	3	ASP	3	THR	4	ARG	4
ARG	3	ARG	3	SER	3	SER	4
THR	3	ASN	3	GLU	3	GLU	4
TYR	3	THR	2	GLN	3	LYS	3
TRP	3	TRP	2	CYS	3	CYS	3
GLN	2	GLN	2	LYS	3	TRP	3
ALA	2	ALA	2	GLY	2	ASN	2
GLU	2	GLU	2	ASP	2	ASP	2
LYS	2	LYS	2	LEU	2	LEU	2
HIS	2	HIS	1	TRP	2	ILE	2
MET	2	MET	1	MET	2	GLN	1
CYS	2	TYR	1	ALA	1	ALA	1
ASN	2	SER	1	TYR	1	TYR	1
PHE	1	PHE	1	VAL	1	VAL	1
PRO	1	PRO	1	ILE	1	HIS	1
VAL	1	VAL	1	HIS	1		
LEU	1	LEU	1				
		ILE	1				
Total AA	**43**		**36**		**43**		**44**
Polar AA	**31**		**20**		**29**		**24**

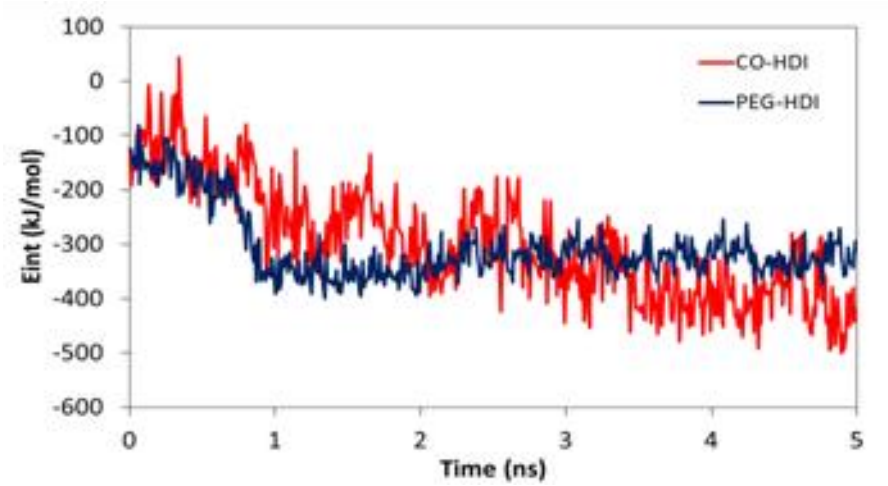

Figure S4. Equilibration of the protein-surface interaction energy on CO-HDI and PEG-HDI surfaces.

References

1. Sirkecioglu, A.; Mutlu, H.; B., Citak, C.; Koc, A.; Guner, F. S. Physical and surface properties of polyurethane hydrogels in relation with their chemical structure. *International Polymer Science*, **2012**, submitted.
2. Hou,, Y.; Tang, J.; Zhang, H.; Qian, C.; Feng, Y.; and Liu, J. Functionalized Few-Walled Carbon Nanotubes for Mechanical Reinforcement of Polymeric Composites, *National Institute for Materials Science*, **2009**, *3*, 1057–1062.
3. Ma, P. X. and Elisseeff, J.,: Scaffolding in tissue engineering. CRC Press, USA, 2006.
4. Damas, C.; Leprince, T.; Ngo, T. H. V.; Coudert, R.: Behavior study of polyvinyl alcohol aqueous solutionin presence of short chain micelle-forming polyols, *Colloid Polymer Science,* **2008**, *286*, 999-1007.
5. Ebewele, R. O. Polymer Science and Technology. CRC press, USA, 2000.