Supplementary Material for

Molecular Simulation of Fibronectin Adsorption onto Polyurethane Surfaces

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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

<table>
<thead>
<tr>
<th>Property</th>
<th>Method</th>
<th>PVA</th>
<th>CO-HDI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young modulus (GPa)</td>
<td>This work</td>
<td>5.43</td>
<td>1.76</td>
</tr>
<tr>
<td></td>
<td>Experimental [2]</td>
<td>4.34 +/- 0.017</td>
<td></td>
</tr>
<tr>
<td>Poisson ratio</td>
<td>This work</td>
<td>0.31</td>
<td>0.37</td>
</tr>
<tr>
<td></td>
<td>Experimental [3]</td>
<td>0.426-0.447</td>
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</tr>
<tr>
<td>Radius of gyration (Å)</td>
<td>This work</td>
<td>8.17</td>
<td>16.61</td>
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<tr>
<td></td>
<td>Experimental [4]</td>
<td>11.4</td>
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<tr>
<td>Cohesive energy density (cal/cm³)</td>
<td>This work</td>
<td>138.87</td>
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<tr>
<td></td>
<td>Experimental [4]</td>
<td>158-201</td>
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</tr>
<tr>
<td>Solubility parameter (cal/cm³)¹/²</td>
<td>This work</td>
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<td>Experimental [4]</td>
<td>12.6-14.2</td>
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**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 $\delta = 7\text{Å}$ 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 $E_{\text{int}}$ (kJ/mol) and strain energies $E_{\text{strain}}$ (kJ/mol) after energy minimization as function of the adsorption layer thickness ($\delta$) based on the number of amino acids ($N_{\text{AA}}$) and on the number of protein atoms ($N_{\text{Atom}}$).

<table>
<thead>
<tr>
<th>E$_{\text{int}}$ (kJ/mol)</th>
<th>$N_{\text{AA}}$</th>
<th>$N_{\text{Atom}}$</th>
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<tr>
<td></td>
<td>$\delta = 3 \text{ Å}$</td>
<td>$\delta = 5 \text{ Å}$</td>
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<tr>
<td>PEG</td>
<td>25.01</td>
<td>19.66</td>
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<tr>
<td>PVA</td>
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<tr>
<td>PEG-HDI</td>
<td>28.23</td>
<td>20.10</td>
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<td>CO-HDI</td>
<td>23.93</td>
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<tr>
<th>E$_{\text{strain}}$ (kJ/mol)</th>
<th>$\delta = 3 \text{ Å}$</th>
<th>$\delta = 5 \text{ Å}$</th>
<th>$\delta = 7 \text{ Å}$</th>
<th>$\delta = 3 \text{ Å}$</th>
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<td>5.84</td>
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<td>3.50</td>
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<td>1.29</td>
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<td>PEG-HDI</td>
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<td>CO-HDI</td>
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<td>3.38</td>
<td>2.54</td>
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<td>0.21</td>
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</table>

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

<table>
<thead>
<tr>
<th>PEG-HDI Orientation</th>
<th>Orientation</th>
<th>CO-HDI Orientation</th>
<th>Orientation</th>
<th>PEG Orientation</th>
<th>Orientation</th>
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<tr>
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Figure S4. Equilibration of the protein-surface interaction energy on CO-HDI and PEG-HDI surfaces.

References


