The interaction with gold suppresses fiber-like conformations of the Amyloid β (16-22) peptide

Luca Bellucci, a,b Albert Ardèvol, c,d Michele Parrinello, c,d Helmut Lutz, e Hao Lu, e Tobias Weidner e and Stefano Corni b,d

Table S1 Summary of XPS determined elemental composition for Aβ16-22 on the Au surface. Values in atomic % with experimental errors in parentheses.

<table>
<thead>
<tr>
<th></th>
<th>O</th>
<th>N</th>
<th>C</th>
<th>Au</th>
</tr>
</thead>
<tbody>
<tr>
<td>Composition</td>
<td>7.4(0.9)</td>
<td>4.8(0.6)</td>
<td>40.0(0.8)</td>
<td>47.8(1.9)</td>
</tr>
<tr>
<td>Composition omitting Au</td>
<td>16.6(0.1)</td>
<td>10.1(0.2)</td>
<td>73.3(0.5)</td>
<td>-</td>
</tr>
<tr>
<td>Theoretical</td>
<td>16.4</td>
<td>13.1</td>
<td>70.5</td>
<td>-</td>
</tr>
</tbody>
</table>

a Dipartimento FIM, Università di Modena e Reggio Emilia, I-41125, Modena, Italy; E-Mail: luca.bellucci_s3@unimore.it
b Centro S3, CNR-NANO Istituto Nanoscienze, I-41125, Modena, Italy; E-Mail: stefano.corni@nano.cnr.it
c Department of Chemistry and Applied Biosciences, ETH-Zurich, Switzerland.
d Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera italiana, CH-6900, Lugano, Switzerland
e Max Planck Institute for Polymer Research, D-55128 Mainz, Germany
†Electronic Supplementary Information (ESI) available: representative structures for the most populated conformational structures of Aβ16-22 on bulk and on the metal surface. Normalized distribution of the variable s defined as the sum of internal dihedral angles of the peptide in solution and at the gold/water interface. See DOI: 10.1039/b000000x/
Upper panels: representative structures for the most populated conformational basins for Aβ₁₆₋₂₂ in bulk solution and on the surface. For each basin, the backbones of various structures chosen randomly among the basin populations are superimposed and displayed together to show the internal conformational homogeneities within a given basin. Lower panels: percentage populations of representative basins, obtained by integrating the population density over a radius of 2 units from the local density maximum.

Sketch-map for Aβ₁₆₋₂₂ in (a) bulk solution and (b) on the surface. These are zooms of panels (a) and (b), respectively, of Fig. 4 in the main text. The same colour scale as in the main text is used. Spots labeled 1 and 2 are kept to allow to better identify these zooms in the original maps. The black crosses show the position of experimental fiber structures in the sketch-map space. Since the experimental structures lack the last amino acid, we have assumed for the corresponding backbone angles those for an ideal β-strand (150° and -80°), for Φ of residue A and Ψ of residue E, respectively. It is apparent that the experimental fibers correspond to a region that is much less populated on the surface than in bulk water.
Fig. S3 (a) Comparison between the calculated (top) and the experimental (bottom) SFG spectra of Aβ₁₆₋₂₂. The calculated spectra are obtained for a structure on the surface (“Surface”, solid line, see main text) and the three representative bulk structures shown in panel b (“Bulk”, dashed lines). The calculated surface spectrum agrees better with the experimental data than those calculated from bulk structures. In particular, structure 2 is quite close to fiber, with a similarity index $s \approx 9$. (b) Snapshots of the simulated bulk structures used for the spectra calculations. They have been oriented on the surface by aligning them to the conformationally closest structure in the surface conformational ensemble of the peptide.