Journal Name

ARTICLE TYPE

Cite this: DOI: 10.1039/xxxxxxxxxx

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

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Received Date
Accepted Date

DOI: 10.1039/xxxxxxxxxx

www.rsc.org/journalname

Table S1 Summary of XPS determined elemental composition for Aβ_{16-22} on the Au surface. Values in atomic % with experimental errors in parentheses.

	O	N	C	Au
Composition	7.4(0.9)	4.8(0.6)	40.0(0.8)	47.8(1.9)
Composition omitting Au	16.6(0.1)	10.1(0.2)	73.3(0.5)	-
Theoretical	16.4	13.1	70.5	-

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†Electronic Supplementary Information (ESI) available: representative structures for the most populated conformational structures of Aβ_{16-22} 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/

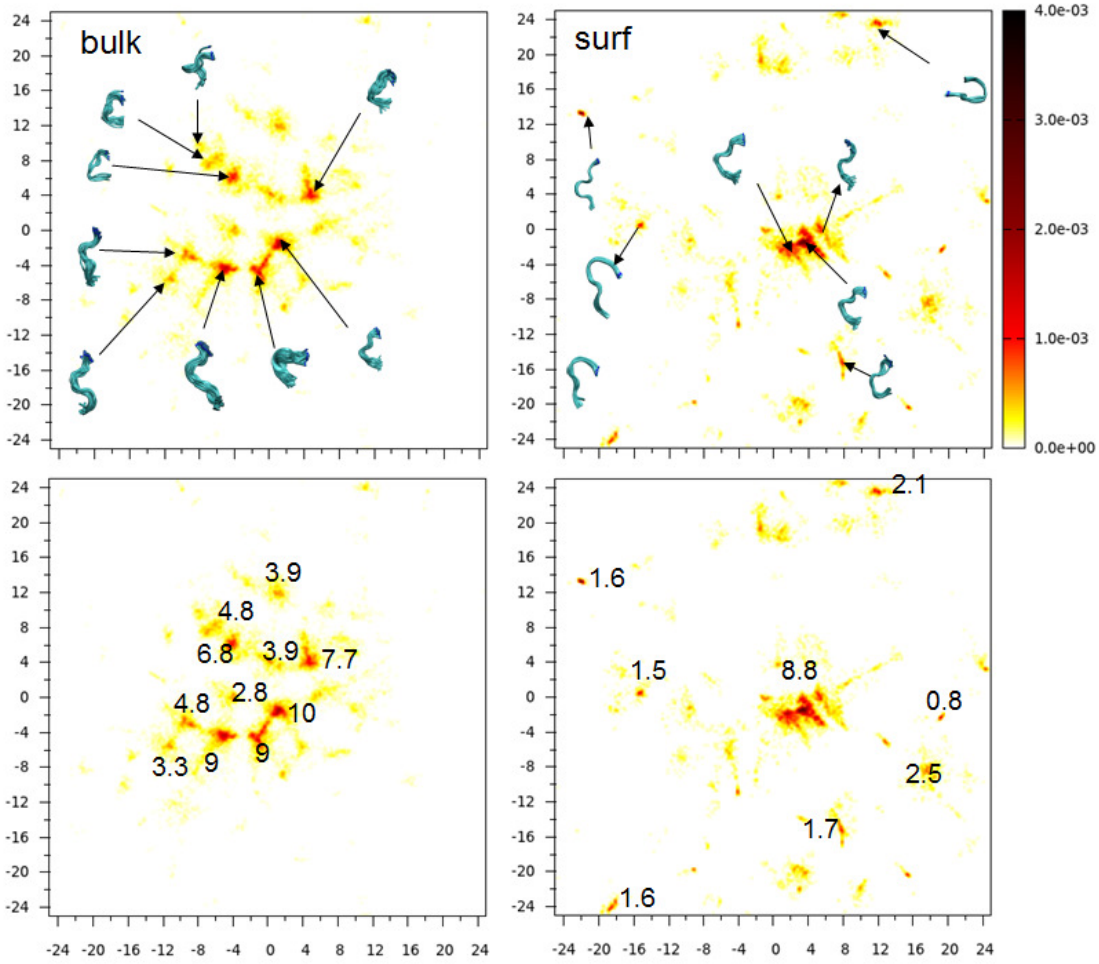

Fig. S1 Upper panels: representative structures for the most populated conformational basins for Aβ_{16-22} in bulk solution and on the surface. For each basin, the backbones of various structures chosen randomly among the basin populations are superimposed and displayed together to show the internal conformational omogeneities 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

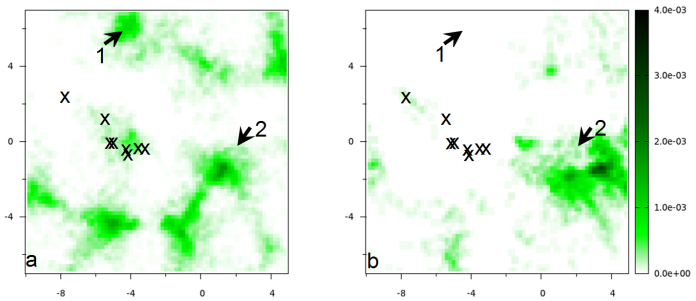

Fig. S2 Sketch-map for Aβ_{16-22} in (a) bulk solution and (b) on the surface. These are zooms of panels (a) and (b), respectively, of Fig. 4 in the main text. The same colour scale as in the main text is used. Spots labeled 1 and 2 are kept to allow to better identify these zooms in the original maps. 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^o and -80^o), 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

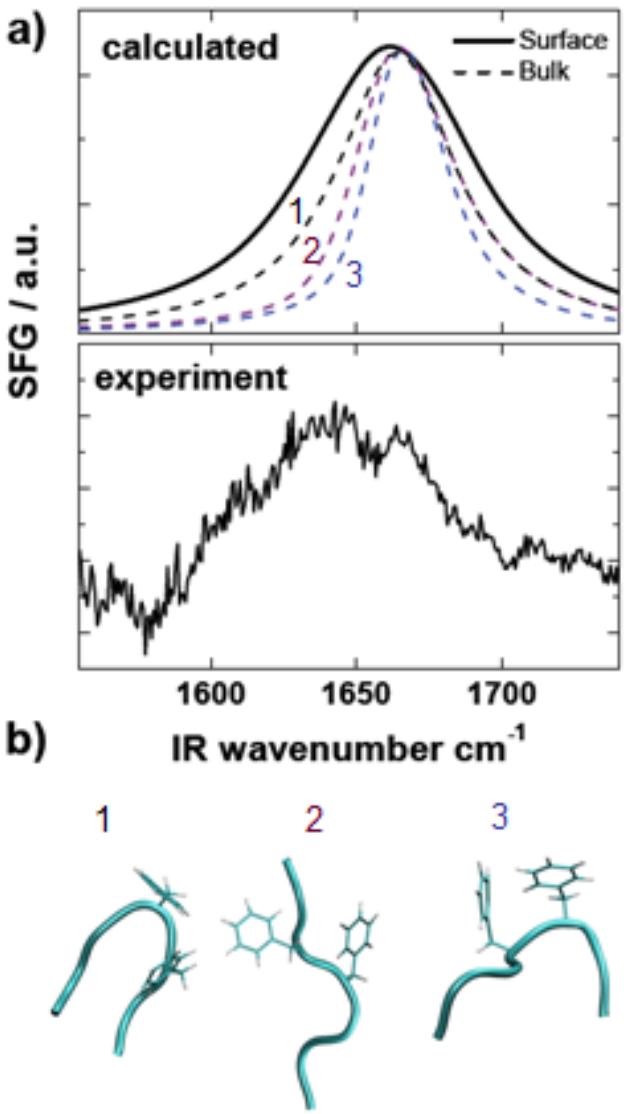

Fig. S3 (a) Comparison between the calculated (top) and the experimental (bottom) SFG spectra of Aβ_{16-22}. The calculated spectra are obtained for a structure on the surface ("Surface", solid line, see main text) and the three representative bulk structures shown in panel b ("Bulk", dashed lines). 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.