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Supplementary Information for

Functionalizing gold with single strand DNA: novel insight into optical properties via combined Spectroscopic Ellipsometry and nanolithography measurements

Giulia Pinto[a], Pietro Parisse[b*], Ilaria Solano[a], Paolo Canepa[a], Maurizio Canepa[a], Loredana Casalis[b], Ornella Cavalleri[a*]

SE dynamic spectra were recorded to monitor the addition of MCH. Figure S1 shows the SE dynamic Ψ spectra in the UV and in the NIR after addition of MCH.

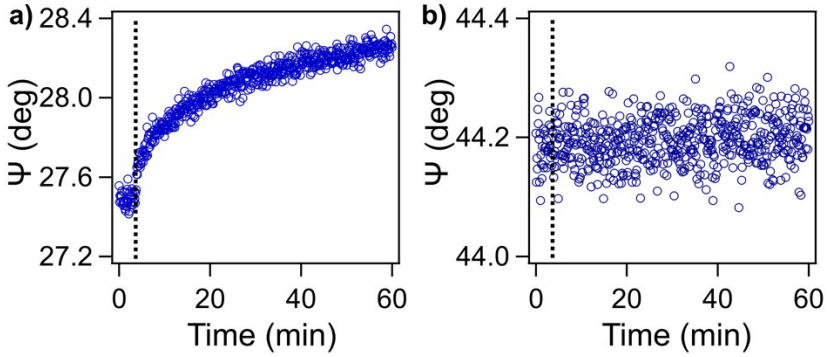

Figure S1 SE dynamic Ψ spectra at (a) 350 nm and (b) 800 nm. The dotted line marks the injection of MCH in the cell.

C_6-ssDNA data have been analysed through the comparison with simulations based on a 3-layer model (ambient|layer|substrate) (Fig. S2a-b) and on a 4-layer model (ambient|layer|interface|substrate) (Fig. S2c-d).
Within the 3-layer model, assuming the AFM thickness of the C_6-ssDNA layer (d_L=3 nm) as reference, we obtained a satisfactory agreement between C_6-ssDNA $\delta_1\Delta$ experimental data (red crosses) and simulations using A=1.42 (B=0.003 μm^2) (Fig. S2a). Curves calculated with the same A and B values but changing the film thickness (d_L=2 nm and 4 nm) are shown for useful comparison. We note that, as expected, the 3-layer model can not account for negative $\delta_1\Psi$ values (Fig. S2b).
Simulations obtained with the 4-layer model allow to reproduce the negative $\delta_1\Psi$ values (Fig. S2d), indicating the importance of the interface layer for a reliable optical modelling of the system. Within the 4-layer model a very low index mismatch between film and ambient (A~1.30) is required. Assuming the AFM thickness (d_F=3 nm) as reference, A values between 1.30 and 1.31 should be needed to reproduce $\delta_1\Delta$ experimental data (Fig. S2c).

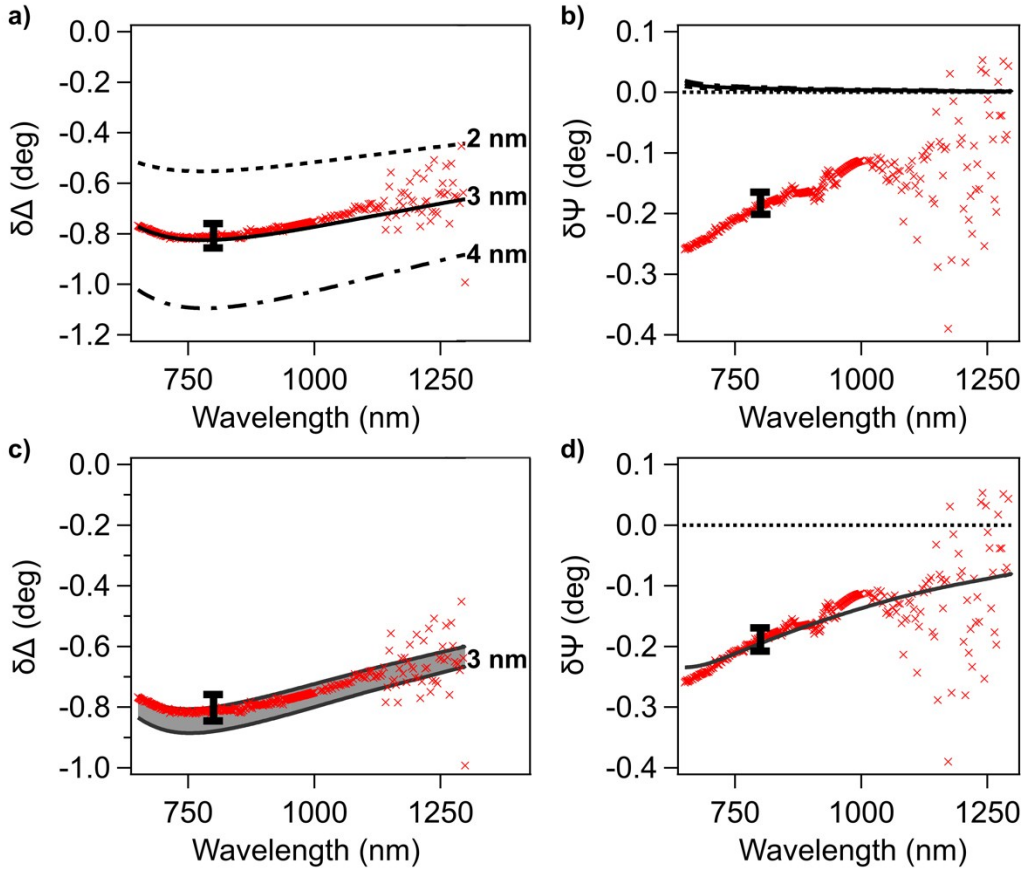

Figure S2 (a-b) Comparison between NIR SE δ-data for C_6-ssDNA (red crosses) and simulations (black lines) obtained with the 3–layer model: A=1.42, B=0.003 μm² and for d_L=2 nm, 3 nm and 4 nm. (c-d) Comparison between NIR SE δ-data for C_6-ssDNA (red crosses) and simulations (black lines) obtained with the 4-layer model for d_F=3 nm and Cauchy A-coefficient values comprised between 1.30 (top border) and 1.31 (bottom border), B=0.02 μm². Error bars take into account the sample to sample variability (about 20%).

Figure S3 shows the refractive index of the Cauchy layer used in the 4-layer simulations for C_6-ssDNA/MCH film.

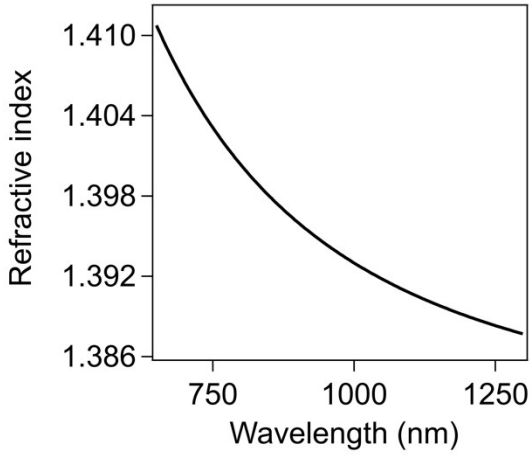

Figure S3 Refractive index in 650-1300 nm range for a Cauchy film with A=1.38 and B=0.013 μm² (parameters used for the 4-layer simulation of the C_6-ssDNA/MCH film).

Figure S4 compares the experimental data for C_6-ssDNA SAM and C_6-ssDNA/MCH SAM with a 4-layer simulation (d_F=1 nm, A=1.47), which is intended to model an ideally compact MCH layer (green dashed line). The comparison indicates that exposure to MCH does not simply results in the replacement of weakly bound ss-DNA by MCH but promotes reorganization in the whole film.

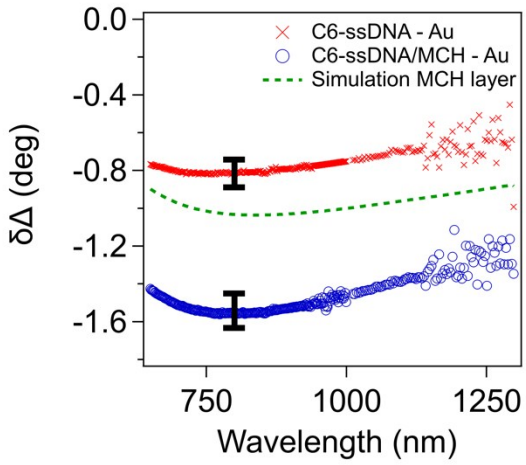

Figure S4 Comparison between NIR SE δ-data for C_6-ssDNA (red crosses), C_6-ssDNA/MCH (blue circles) and simulation for a MCH layer (d_F=1 nm, A=1.47, B=0.013 μm^2). Error bars take into account the sample to sample variability (about 20% for C_6-ssDNA, about 25% for C_6-ssDNA/MCH).