coatings

MDPI

Supplementary

Surface Chemistry, Crystal Structure, Size and Topography Role in the Albumin Adsorption Process on TiO_2 Anatase Crystallographic Faces and Its 3D-Nanocrystal: A Molecular Dynamics Study †

Giuseppina Raffaini [1,2]

[1] Department of Chemistry, Materials, and Chemical Engineering "Giulio Natta", Politecnico di Milano, Piazza L. Da Vinci 32, 20131 Milano, Italy; giuseppina.raffaini@polimi.it

[2] INSTM, National Consortium of Materials Science and Technology, Local Unit Politecnico di Milano, 20131 Milano, Italy

† Dedicated to the memory of my father Mario Tancredi Raffaini

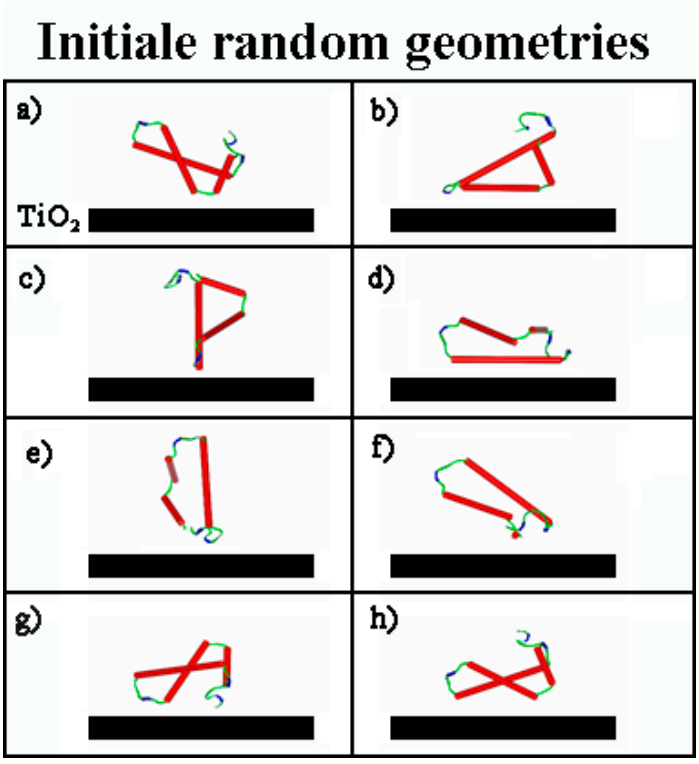

Figure S1. Scheme of the eight different initial *non-optimized* geometries studied in the *Section 3.1.1*, considering the three α-helices of the HSA *A*-subdomain considered near the TiO_2 anatase surface, using a simulation protocol proposed in previous work [1].

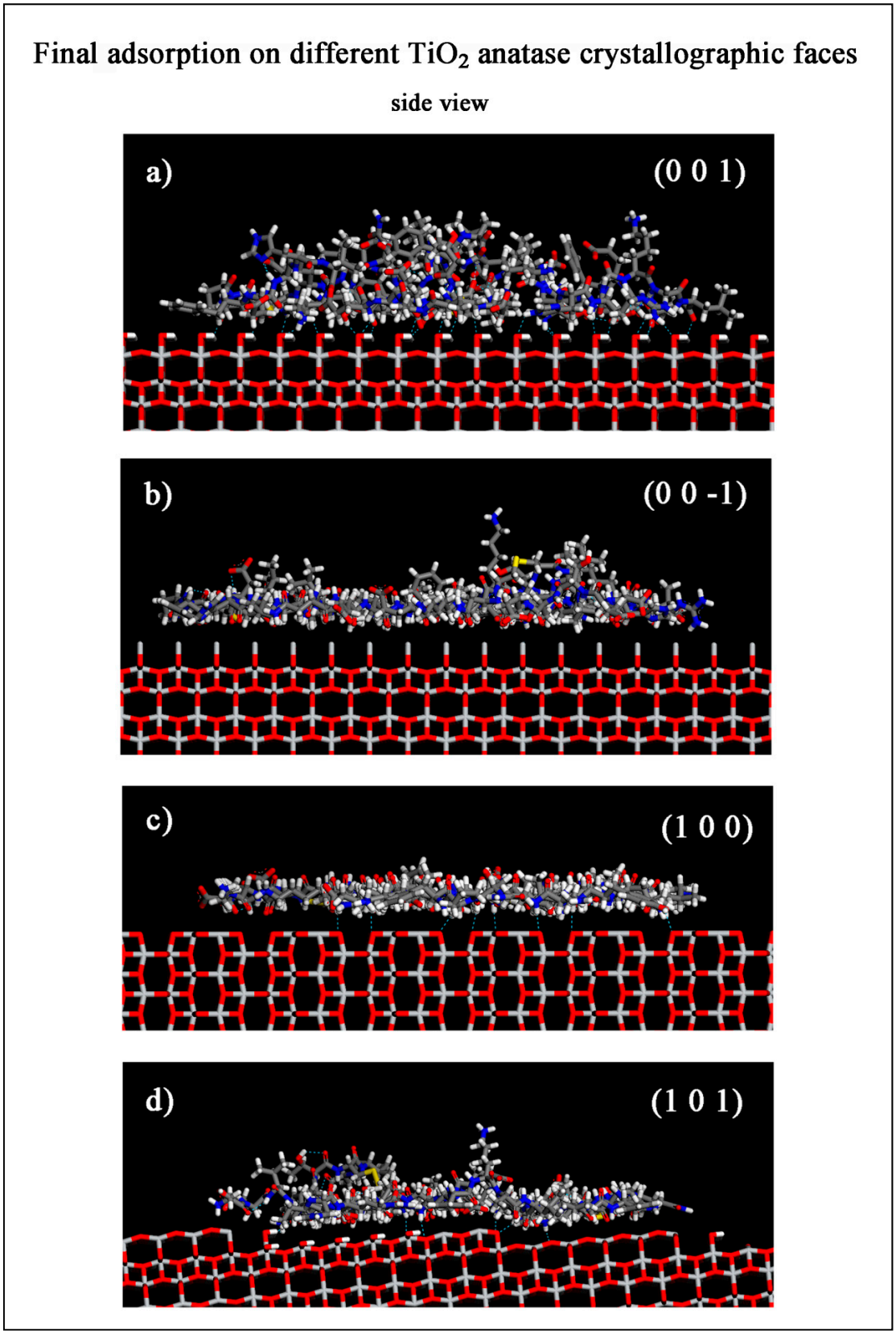

Figure S2. The Albumin *A*-subdomain in the final adsorption stage on the four different TiO_2 crystallographic faces reported in Figure 5, displaying the H-bonds between the protein fragment and the solid surface.

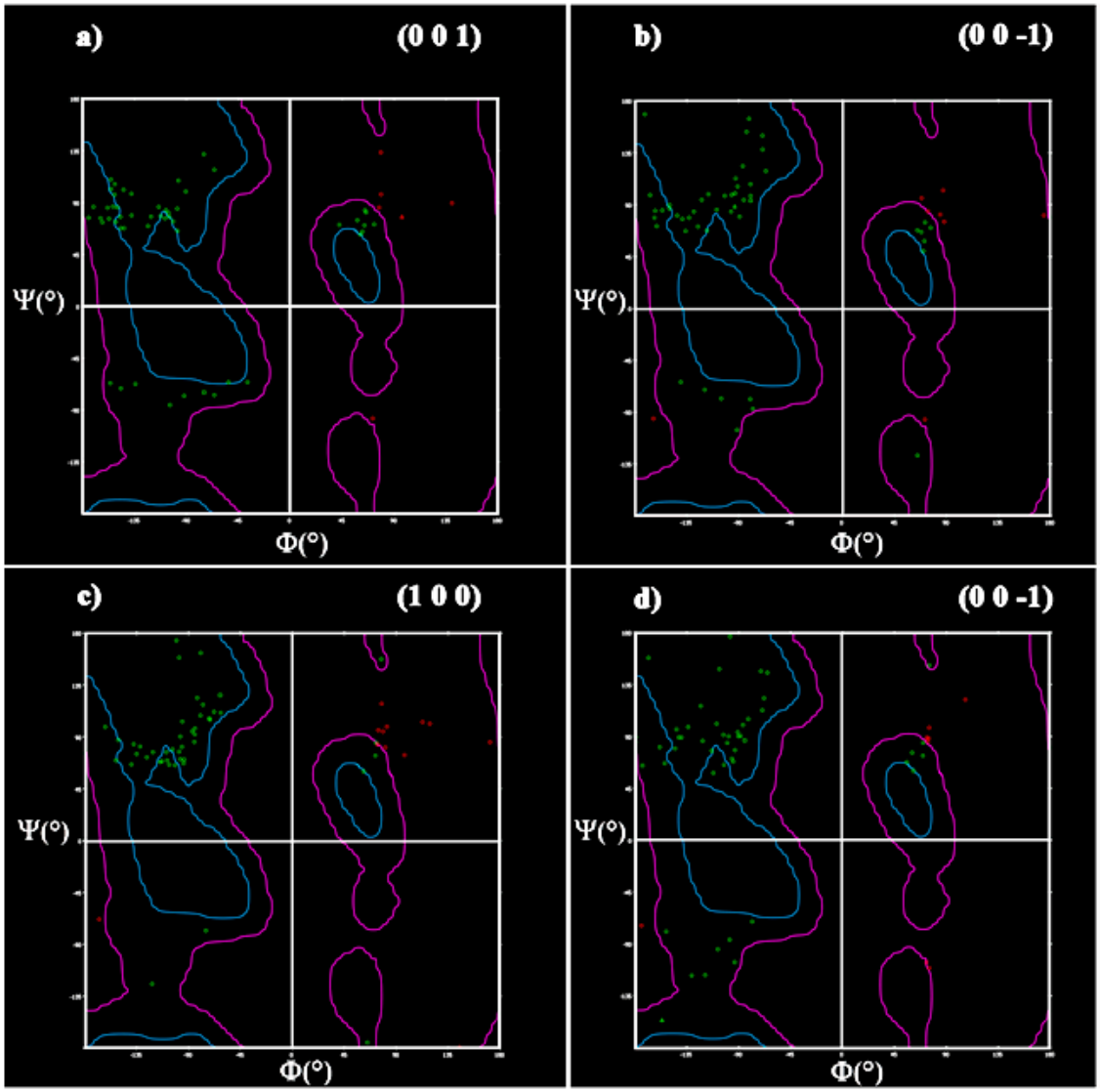

Figure S3. The Ramachandran Plot of the albumin *A*-subdomain in the final adsorption stage on the four different TiO_2 crystallographic faces reported in Figure 5.

Reference

1. Raffaini, G.; Ganazzoli, F. Simulation study of the interaction of some albumin subdomains with a flat graphite surface. *Langmuir* **2003**, *19*, 3403–3412, doi:10.1021/la026853h.