Electronic supplementary information

Eutectic Liquid Crystal Mixture E7 in Nanoporous Alumina. Effect of Confinement on the Thermal and Concentration Fluctuations.

Aristoula Selevou, [a] George Papamokos, [a] Tolga Yildirim, [c] Hatice Duran [c]

Martin Steinhart [d] and George Floudas*[a,b]

[a] Department of Physics, University of Ioannina, P.O. Box 1186, 451 10 Ioannina, Greece

[b] University Research Center of Ioannina (URCI) - Institute of Materials Science and Computing

[c] Department of Materials Science & Nanotechnology Engineering, TOBB University of Economics and Technology, Söğütözü Cad. 43, Ankara, 06560, Turkey

[d] Institut für Chemie neuer Materialien, Universität Osnabrück, D-49069 Osnabrück, Germany

(A) AAO pore surface modification with ODPA.

XPS was used to determine the surface composition of porous AAO before and after modification of inner walls with ODPA. The carbon and phosphorous amount increased on ODPA modified AAO membrane (Figure S1A to S1F). Examination of the C1s which appears at around 285 eV indicates that carbonaceous contaminants (i.e. COX, CO and C(O)OX) were present on the native AAO surface (Figure S1A). These decreased in intensity after modifying the interface with ODPA, but C–OX environments were still observed at a significant concentration. It is illustrative to compare the carbon and phosphorous concentrations to those of a fully formed ODPA monolayer on the AAO. Hence, for further confirmation of ODPA attachment on the AAO surface, atomic % were analyzed by angle-resolved XPS with shallow probing depths of 2–3 nm at 60° take off angle is shown in Table S1. For empty AAO, the oxygen concentration was 53 at.% and Al was 36 at.%, with 11 at.% of C due to a carbonaceous contamination over layer. In the presence of ODPA, an attenuation of signal from the Al elements present in native AAO membranes, and the appearance of P peaks due to ODPA layer formation is confirmed. On the other hand, carbon/phosphorus (C/P) ratio for pristine samples of ODPA is close to those reported in the literature[1]. The increase in C and P intensities and decrease in Al intensities indicates successful attachment of ODPAs to the oxide surface (Table S1 and Figure S1E).

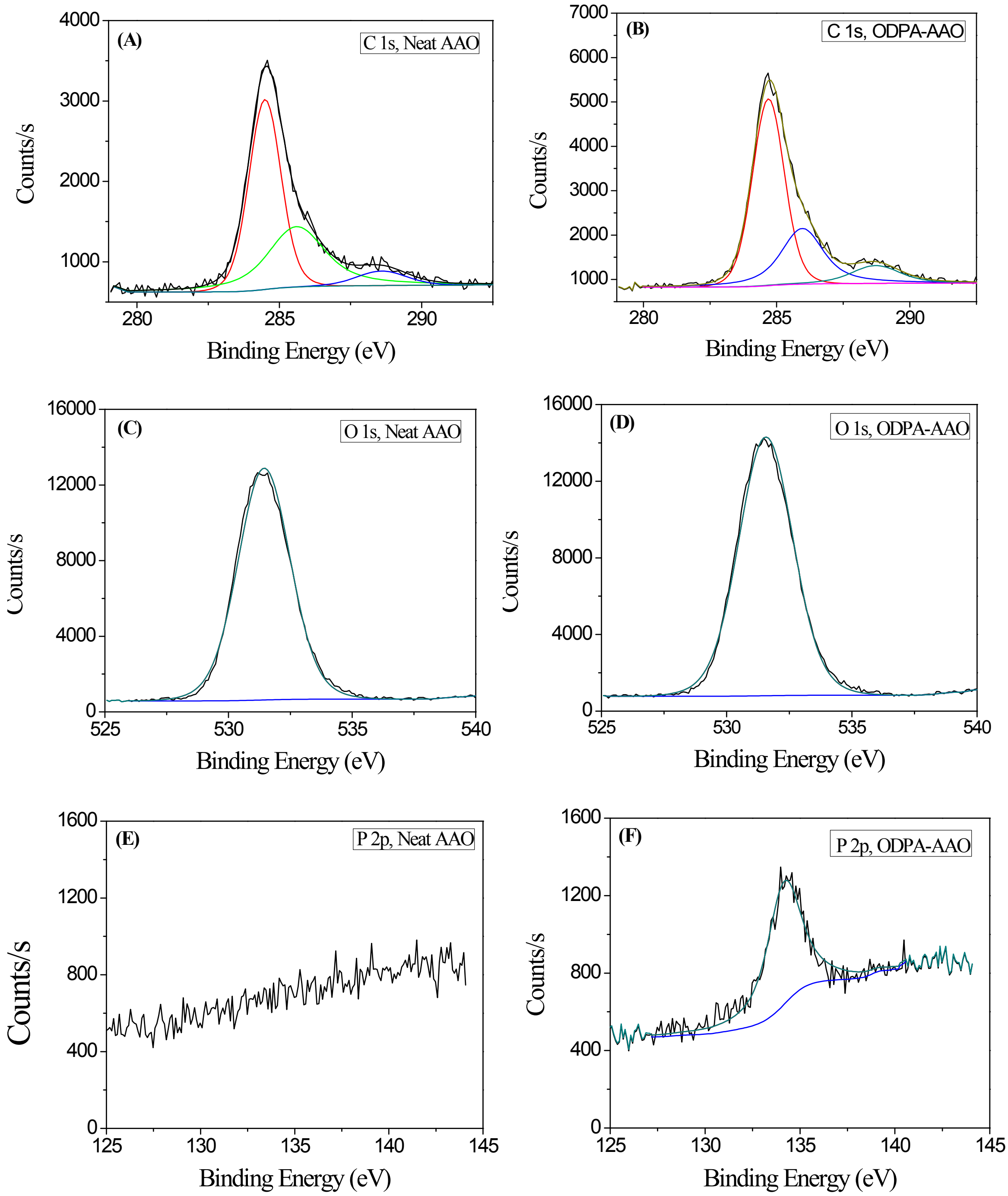

Fig. S1 XPS high-resolution spectra for both reference native AAO with 25 nm in diameter and ODPA samples for (A)-(B) C 1s, (C)-(D) O1s, (E)-(F) P 2p.

Table S1. Total Atomic % of native AAO and ODPA Modified AAO with 25 nm in diameters determined from XPS spectra

	C 1s	O 1s	Al 2p	P 2p
Native AAO (25 nm)	10.94	53.09	35.96	0
ODPA-AAO	37.99	36.3	22.04	3.67

(B) Cartesian Coordinates of the optimized structures of this work B3LYP/cc-pVTZ

5CB

N	7.731212	0.559340	0.608518
C	6.596359	0.422543	0.457700
C	5.190960	0.253167	0.270999
C	4.364236	1.365062	0.080284
C	3.003028	1.194397	-0.099639
C	2.422235	-0.080472	-0.096431
C	3.263735	-1.183970	0.095232
C	4.626311	-1.026394	0.276854
C	0.966143	-0.255180	-0.288796
C	0.257296	-1.240694	0.406149
C	-1.108035	-1.401857	0.223631
C	-1.822122	-0.592358	-0.660682
C	-1.113406	0.387045	-1.357790
C	0.250939	0.556558	-1.175604
C	-3.312090	-0.746644	-0.830197
C	-4.125998	0.120759	0.144935
C	-5.636500	-0.037650	-0.027276
C	-6.454182	0.821604	0.938158
C	-7.962902	0.658211	0.761157
H	4.794083	2.356648	0.083821
H	2.374937	2.065891	-0.220301
H	2.847344	-2.181373	0.077065
H	5.261838	-1.889617	0.414603
H	0.774643	-1.873189	1.115083
H	-1.629366	-2.170583	0.780942
H	-1.635586	1.020044	-2.064865
H	0.772698	1.307667	-1.753452
H	-3.591048	-0.486393	-1.854418
H	-3.588578	-1.794557	-0.688875
H	-3.844220	-0.134666	1.170608
H	-3.848331	1.169793	0.006778
H	-5.912540	0.214945	-1.056648
H	-5.908453	-1.089921	0.108276
H	-6.178197	0.569016	1.966300
H	-6.182777	1.872745	0.802103
H	-8.516653	1.283147	1.463073
H	-8.274494	0.937008	-0.247624
H	-8.269816	-0.376755	0.92579 0

7CB

N	-8.692683	-1.153514	0.517992
C	-7.576970	-0.888801	0.397709
C	-6.195298	-0.561006	0.248741
C	-5.325009	-1.444494	-0.397945
C	-3.987090	-1.121272	-0.538829
C	-3.473204	0.084749	-0.044709
C	-4.357759	0.959057	0.600093
C	-5.697607	0.646998	0.747901
C	-2.041768	0.423535	-0.199129
C	-1.345545	1.101580	0.806970
C	-0.003400	1.417981	0.658794
C	0.698916	1.076671	-0.497704
C	0.002412	0.405035	-1.503333
C	-1.338336	0.081298	-1.358866
C	2.166452	1.390271	-0.640752
C	3.079650	0.267976	-0.118863
C	4.567457	0.587699	-0.264552
C	5.482736	-0.523284	0.251976
C	6.971734	-0.206633	0.108019
C	7.888164	-1.316840	0.624062
C	9.373664	-0.991729	0.476304

H	-5.702430	-2.383329	-0.777640
H	-3.323240	-1.826660	-1.018711
H	-3.995042	1.908136	0.969150
H	-6.367482	1.337435	1.240440
H	-1.852623	1.363971	1.725829
H	0.509046	1.938611	1.458585
H	0.514502	0.141717	-2.420791
H	-1.853189	-0.414963	-2.170623
H	2.398390	1.576361	-1.692494
H	2.396091	2.313719	-0.103117
H	2.845811	0.077266	0.932589
H	2.848545	-0.658021	-0.653392
H	4.794012	0.782040	-1.318202
H	4.791290	1.517606	0.268772
H	5.255219	-0.717544	1.305355
H	5.258222	-1.452868	-0.281493
H	7.200170	-0.012306	-0.945412
H	7.197202	0.722938	0.641606
H	7.660516	-1.510783	1.676614
H	7.663586	-2.245446	0.090606
H	9.999282	-1.802185	0.852895
H	9.639377	-0.827082	-0.570045
H	9.636336	-0.086772	1.028218

5CT

N	9.873541	0.330959	0.618762
C	8.728024	0.269593	0.503211
C	7.309442	0.193623	0.360114
C	6.611316	-0.926127	0.823813
C	5.236691	-0.993784	0.682531
C	4.514748	0.043926	0.078370
C	5.228620	1.158543	-0.381036
C	6.603158	1.238146	-0.245152
C	3.046039	-0.034766	-0.069605
C	2.241855	1.102662	0.061427
C	0.865332	1.027804	-0.074628
C	0.226614	-0.185893	-0.353473
C	1.032763	-1.322135	-0.486992
C	2.408893	-1.249434	-0.345833
C	-1.243440	-0.264031	-0.501115
C	-1.961257	-1.371146	-0.036612
C	-3.339388	-1.442182	-0.177938
C	-4.059842	-0.415381	-0.788994
C	-3.343543	0.687240	-1.256269
C	-1.965855	0.764721	-1.115068
C	-5.561543	-0.478419	-0.908296
C	-6.292842	0.147960	0.290932
C	-7.815032	0.083056	0.167780
C	-8.550962	0.704768	1.355579
C	-10.071786	0.636194	1.226107
H	7.151087	-1.731990	1.300487
H	4.710160	-1.854797	1.069691
H	4.701680	1.963135	-0.874434
H	7.138679	2.101631	-0.613392
H	2.694888	2.052934	0.310096
H	0.272601	1.920807	0.069800
H	0.578623	-2.271246	-0.737113
H	3.000276	-2.143711	-0.489451
H	-1.438081	-2.176812	0.460971
H	-3.865817	-2.311783	0.196618
H	-3.871086	1.493691	-1.751217
H	-1.440246	1.621757	-1.514626
H	-5.876303	0.032699	-1.821832
H	-5.875792	-1.520249	-1.010866
H	-5.976216	-0.359460	1.206879
H	-5.976831	1.189853	0.397215
H	-8.126104	0.588073	-0.753026
H	-8.125671	-0.961553	0.058369
H	-8.240205	0.200068	2.275245
H	-8.240986	1.748412	1.464270

H	-10.566209	1.087309	2.087504
H	-10.416024	1.162573	0.333402
H	-10.415257	-0.397671	1.150971

8OCB

C	10.902881	-0.361156	0.059275
H	11.697933	-1.094962	0.198707
C	-0.836001	-0.526910	0.122337
C	-2.206935	-0.752060	0.156911
C	-3.128506	0.274743	-0.053844
C	-2.618276	1.556969	-0.307492
C	-1.259393	1.796353	-0.351354
C	-0.350894	0.755525	-0.135020
H	-0.162168	-1.349520	0.305270
H	-2.559959	-1.749298	0.382822
H	-3.298645	2.374997	-0.501999
H	-0.873612	2.784136	-0.561321
C	-4.583493	0.023049	-0.010282
C	-5.468497	0.978848	0.507397
C	-6.832042	0.749511	0.551165
C	-7.356634	-0.456850	0.075789
C	-6.487161	-1.421720	-0.443510
C	-5.125898	-1.179216	-0.484820
H	-5.079457	1.905736	0.904987
H	-7.497435	1.495668	0.961809
H	-6.887011	-2.351882	-0.821739
H	-4.472923	-1.924868	-0.916307
C	-8.762508	-0.700403	0.119596
N	-9.898089	-0.897467	0.155107
O	0.962767	1.089160	-0.194898
C	1.950205	0.076549	0.003612
H	1.821610	-0.714655	-0.742483
H	1.826203	-0.369891	0.995837
C	3.316872	0.721797	-0.127600
H	3.396433	1.526825	0.606943
H	3.391054	1.188028	-1.113031
C	4.456328	-0.279560	0.065948
H	4.361489	-1.087379	-0.667097
H	4.366289	-0.750415	1.050381
C	5.842288	0.354365	-0.062316
C	6.988131	-0.640119	0.127359
H	5.938282	1.161498	0.671072
H	5.932311	0.827050	-1.045684
H	6.890758	-1.447243	-0.606409
H	6.896507	-1.113371	1.110712
C	8.374548	-0.008100	-0.000172
H	8.473217	0.798773	0.733833
H	8.466984	0.465887	-0.983199
C	9.521789	-1.001575	0.188291
H	9.423820	-1.807402	-0.545459
H	9.429940	-1.474840	1.170602
H	11.044071	0.425532	0.803383
H	11.037964	0.090360	-0.925810

References

1. P. Thissen, M. Valtiner, G. Grundmeier, *Langmuir* 2010, **26**, 156.