Supplementary material for article: The Effect of the Electric Field on the α-GPC Interaction with Au(111) Surface: A First Principles Study

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Supporting Information Available

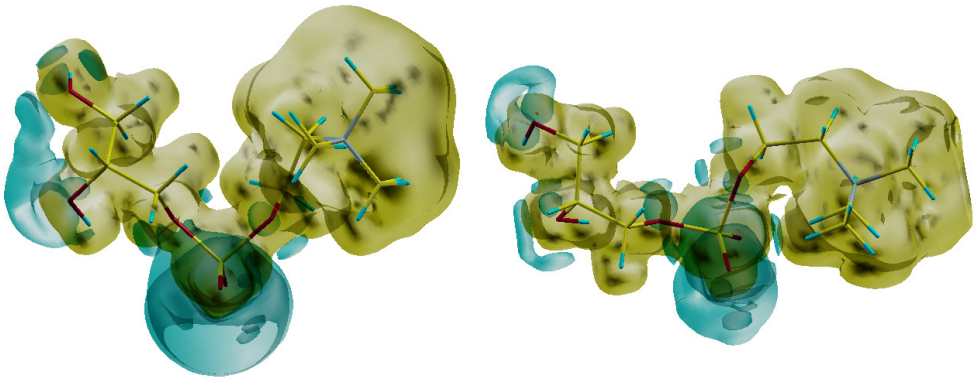

Figure S1: The geometric structures of the α-GPC and the contour plot of Hartree potential plotted at $V_H(\vec{r}) = 0.15V$. RPBE functional was used. Blue/green represents the positive/negative potential values, respectivelly.

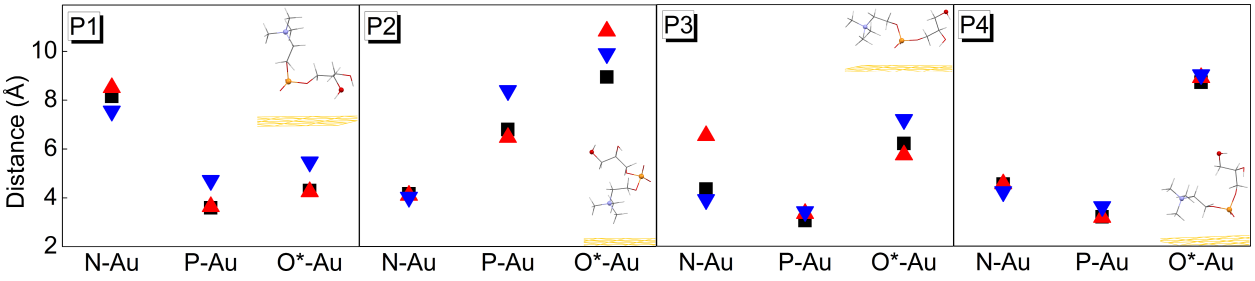

Figure S2: The distance between P, N and the terminal O atom in glycerol $O*$ and Au(111) surface, computed by using RPBE functional. The black square represents the value for the uncharged system while the red and blue triangles represents the electric field orientations (positive/negative relative to the OZ axes).

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Table S1: Total binding energies computed as $\Delta\mathscr{E} = E_{tot} - E_{mol} - E_{surf}$ (i.e. the BSSE effect is not removed), the BSSE corrected interaction energy (ΔE_1) the deformation energy (ΔE_2) and the sum $\Delta E_3 = \Delta E_1 + \Delta E_2$. Data for zero electric field as well as for the two orientations discussed in the text, symbolized by "+" and "-". The type of exchange-correlation functional used is indicated in the top row. All quantities are expressed in eV.

Functional	RPBE	LMKLL	RPBE			LMKLL		
Model	$\Delta\mathscr{E}$	$\Delta\mathscr{E}$	ΔE_1	ΔE_2	ΔE_3	ΔE_1	ΔE_2	ΔE_3
P1	-0.63	0.74	0.22	0.68	0.90	-0.15	0.57	0.42
P2	-0.69	0.79	-0.11	0.37	0.26	-0.32	0.29	-0.03
P3	-1.62	-1.18	0.44	0.07	0.51	-0.36	0.21	-0.15
P4	-1.52	-0.48	0.20	0.38	0.58	-0.26	0.50	0.24
P1+	-1.42	-0.65	-0.11	0.89	0.78	-0.51	0.62	0.11
P2+	-0.42	-0.19	-0.48	0.36	-0.12	-0.72	0.31	-0.41
P3+	-1.51	-0.78	0.14	0.37	0.51	-0.26	0.25	-0.01
P4+	-1.85	-0.58	-0.06	0.50	0.44	-0.50	0.61	0.11
P1-	-0.12	0.71	0.31	0.17	0.48	-0.16	0.12	-0.04
P2-	-1.89	-1.12	-1.04	0.98	-0.06	-0.93	0.76	-0.17
P3-	-1.41	0.86	0.36	0.04	0.40	-0.22	0.14	-0.08
P4-	-1.48	-0.68	0.21	0.41	0.62	-0.35	0.61	0.26

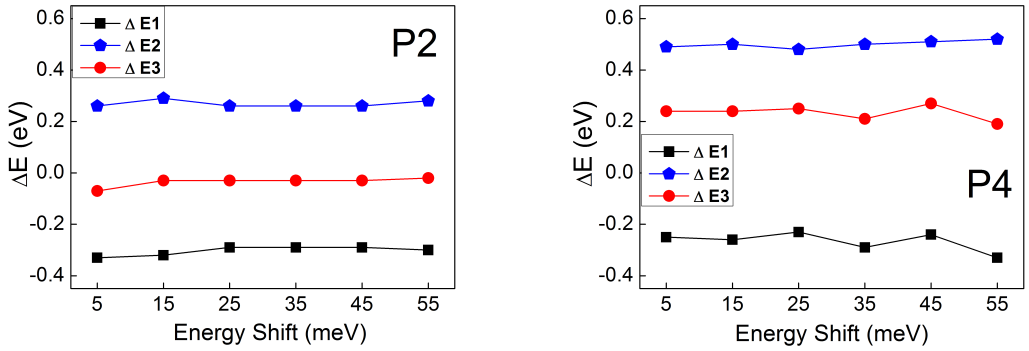

Figure S3: Convergence tests for different basis sets, represented by their energy shift, ε, for orientations P_2 and P_4. For each value of energy shift indicated the system was relaxed, then the energies ΔE_1, ΔE_2 and their sum were computed using Eqs. (2) and (3) in the text.