Supplementary Material (ESI) for PCCP

Supporting Information for
Enantiospecific adsorption of amino acids on hydroxylated quartz $(10\bar{1}0)$

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Below, Table S.1 and S.2 list energetic and structural information for hydroxylated α-quartz $(10\bar{1}0)$ surface upon the adsorption of amino acids, repectively.

Amino Acid		Gly	Ala	Ser	Cys	Asp	Asn
$\mathbf{E_{ad}}$ **(eV)**	***R***	0.71 (0.67)	0.73 (0.72)	0.76 (0.73)	0.81 (0.78)	0.78 (0.76)	0.72 (0.67)
	S		0.75 (0.75)	0.72 (0.70)	0.81 (0.78)	0.88 (0.84)	0.76 (0.71)

Table S.1: Adsorption energies of amino acids in their most stable states on hydroxylated α-quartz $(10\bar{1}0)$. The zero point corrected adsorption energies are also listed in the parentheses.

	SiOH	***d*(O-H) /Å**	***d*(H…O) /Å**	***d*(Si-O) /Å**	**∠(O-H…O) /°**	**∠(Si-O-H) /°**	**carboxyl group** $d(H_{surf}\cdots O_{mole})$/Å $d(O_{surf}\cdots H_{mole})$/Å	**amine group** $d(H_{surf}\cdots N_{mole})$/Å	**side chain** $d(H_{surf}\cdots O_{mole})$/Å $d(O_{surf}\cdots H_{mole})$/Å
Bare surface	**a**	0.98	2.52	1.65	155	116	-	-	-
	b	0.99	1.72	1.62	177	120			
Gly	**1a/b**	0.98, 1.01	2.28, 1.62	1.66, 1.62	158, 178	115, 119	2.61	1.52	-
	2a/b	0.98, 1.00	2.89, 1.69	1.65, 1.61	137, 179	122, 119			
	3a/b	1.07, 1.00	3.25, 1.64	1.62, 1.64	108, 179	124, 120	1.67		-
	4a/b	0.98, 1.00	2.37, 1.71	1.66, 1.62	157, 176	115, 119			
***R*-Ala**	**1a/b**	0.98, 1.01	2.27, 1.61	1.66, 1.62	158, 178	115, 119	2.58	1.50	-
	2a/b	0.98, 0.99	2.90, 1.69	1.65, 1.61	148, 179	122, 119			
	3a/b	1.08, 1.01	3.27, 1.64	1.61, 1.64	107, 179	123, 121	1.65		-
	4a/b	0.98, 0.99	2.36, 1.71	1.65, 1.62	157, 175	115, 119			
***S*-Ala**	**1a/b**	0.98, 1.01	2.28, 1.62	1.66, 1.62	159, 179	115, 119	2.48	1.51	-
	2a/b	0.98, 0.99	2.91, 1.70	1.65, 1.61	148, 179	123, 120			
	3a/b	1.07, 1.00	3.29, 1.63	1.61, 1.64	106, 179	123, 120	1.67		-
	4a/b	0.98, 1.00	2.31, 1.70	1.65, 1.62	158, 173	114, 119			
***R*-Ser**	**1a/b**	0.98, 1.01	2.48, 1.62	1.66, 1.62	152, 179	116, 119	1.86	1.59	-
	2a/b	0.99, 0.99	3.17, 1.72	1.64, 1.61	127, 175	128, 120			
	3a/b	1.05, 1.00	3.64, 1.69	1.62, 1.62	93, 177	122, 121	1.64		1.92
	4a/b	0.98, 1.01	2.30, 1.59	1.65, 1.65	158, 175	116, 117			
***S*-Ser**	**1a/b**	0.99, 1.01	2.24, 1.62	1.66, 1.62	159, 179	115, 119	2.51	1.53	-
	2a/b	0.98, 0.99	2.94, 1.70	1.65, 1.61	147, 179	122, 120			
	3a/b	1.07, 1.01	3.31, 1.63	1.62, 1.64	106, 178	123, 120	1.66		-
	4a/b	0.98, 1.00	2.32, 1.71	1.65, 1.63	157, 173	115, 119			

***R*-Cys**	**1a/b**	0.99, 1.01	2.23, 1.62	1.66, 1.62	159, 179	115, 119	2.45	1.52	-
	2a/b	0.98, 0.99	2.94, 1.70	1.65, 1.61	148, 179	123, 119			
	3a/b	1.07, 1.01	3.30, 1.63	1.62, 1.64	106, 178	123, 120	1.66		-
	4a/b	0.98, 1.00	2.32, 1.71	1.62, 1.62	157, 173	115, 119			
***S*-Cys**	**1a/b**	0.99, 1.01	2.22, 1.63	1.66, 1.62	160, 179	115, 120	2.40	1.54	-
	2a/b	0.98, 0.99	2.99, 1.70	1.65, 1.61	146, 179	123, 120			
	3a/b	1.06, 1.01	3.35, 1.62	1.62, 1.64	104, 179	124, 121	1.63		-
	4a/b	0.98, 1.00	2.30, 1.71	1.65, 1.62	158, 173	115, 119			
***R*-Asp**	**1a/b**	0.98, 1.00	2.38, 1.66	1.66, 1.60	154, 178	115, 121	-	1.68	1.92
	2a/b	0.97, 0.99	3.10, 1.73	1.66, 1.60	135, 173	119, 122			
	3a/b	1.03, 1.01	3.78, 1.61	1.61, 1.64	104, 179	126, 121	1.81		1.55
	4a/b	0.99, 1.00	4.72, 1.66	1.64, 1.65	130, 177	120, 117			
***S*-Asp**	**1a/b**	0.99, 1.00	2.04, 1.69	1.66, 1.60	163, 177	114, 121	1.74	1.65	2.01
	2a/b	0.99, 1.01	2.94, 1.61	1.64, 1.64	142, 171	128, 118			
	3a/b	1.03, 1.01	4.10, 1.58	1.62, 1.64	112, 178	125, 119	1.56		1.61
	4a/b	1.00, 1.00	4.47, 1.70	1.64, 1.63	137, 171	123, 117			
***R*-Asn**	**1a/b**	0.98, 1.01	2.42, 1.60	1.66, 1.60	156, 177	115, 125	-	1.61	1.91
	2a/b	0.98, 1.00	2.49, 1.71	1.66, 1.63	160, 177	114, 121			
	3a/b	1.04, 0.99	4.13, 1.71	1.62, 1.63	112, 176	121, 119	1.74		2.17
	4a/b	1.00, 0.99	3.11, 1.72	1.64, 1.63	125, 175	121, 118			
***S*-Asn**	**1a/b**	0.99, 1.00	2.05, 1.66	1.66, 1.60	165, 177	114, 122	1.81	1.61	1.98
	2a/b	0.99, 1.01	3.05, 1.64	1.64, 1.64	137, 170	128, 119			
	3a/b	1.04, 1.00	4.06, 1.62	1.62, 1.62	114, 177	122, 119	1.58		1.95
	4a/b	0.99, 1.00	4.56, 1.69	1.64, 1.64	130, 173	123, 117			

Table S.2: Selected bond lengths or angles of the DFT-optimized geometries of adsorbed amino acids on hydroxylated α-quartz $(10\bar{1}0)$. Structural information for the bare surface is also included.