Enantiospecific adsorption of amino acids on hydroxylated quartz (0001)

Supporting Information

Jeong Woo Han and David S. Sholl

*School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, 311
Ferst Dr., Atlanta, GA 30332-0100, USA*

Below, Table S.1 lists key structural information for hydroxylated α -quartz (0001) surface upon the adsorption of the amino acids we studied. Structural information for the bare surface is also included.

	Si(OH) ₂	$d(\text{O-H})$ /Å	$d(\text{H...O})$ /Å	$d(\text{Si-O})$ /Å	$\angle(\text{O-H...O})$ /°	$\angle(\text{Si-O-H})$ /°	carboxyl group $d(\text{H}_{\text{surf}}\dots\text{O}_{\text{mole}})/\text{\AA}$ $d(\text{O}_{\text{surf}}\dots\text{H}_{\text{mole}})/\text{\AA}$	amine group $d(\text{H}_{\text{surf}}\dots\text{N}_{\text{mole}})/\text{\AA}$ $d(\text{O}_{\text{surf}}\dots\text{H}_{\text{mole}})/\text{\AA}$	hydroxyl group $d(\text{H}_{\text{surf}}\dots\text{O}_{\text{mole}})/\text{\AA}$ $d(\text{O}_{\text{surf}}\dots\text{H}_{\text{mole}})/\text{\AA}$
Bare surface		0.99, 0.98	1.81, 2.37	1.62, 1.65	173, 162	119, 114	-	-	-
Gly	1	1.00, 0.99	1.85, 1.93	1.62, 1.65	166, 167	118, 112	1.85	1.58	-
	2	0.99, 1.00	1.74, 1.85	1.64, 1.64	175, 171	118, 113			
	3	1.01, 0.99	1.68	1.63, 1.63	175	120, 125	1.77	2.14	-
	4	0.99, 1.06	1.74	1.64, 1.63	175	119, 113			
Gly (less stable)	1	1.01, 0.99	1.82, 1.94	1.63, 1.65	175, 172	117, 112	1.78	1.56	-
	2	0.99, 1.00	1.63, 1.81	1.63, 1.65	172, 172	121, 113			
	3	1.00, 1.06	1.73	1.64, 1.62	177	121, 123	1.92	2.06	-
	4	1.01, 0.99	1.62	1.63, 1.65	175	121, 114			
R-Ala	1	0.99, 0.99	1.86, 1.91	1.62, 1.65	165, 167	119, 112	1.87	1.59	-
	2	0.99, 1.00	1.75, 1.89	1.64, 1.64	176, 171	118, 113			
	3	1.00, 0.99	1.69	1.63, 1.64	176	121, 126	1.78	2.17	-
	4	1.00, 1.05	1.73	1.64, 1.63	178	119, 113			
S-Ala	1	1.01, 0.99	1.82, 1.93	1.63, 1.65	173, 169	116, 112	1.74	1.61	-
	2	0.99, 1.00	1.61, 1.82	1.62, 1.65	173, 172	122, 114			
	3	1.00, 1.05	1.73	1.64, 1.62	176	120, 127	1.86	2.16	-
	4	1.01, 1.00	1.64	1.63, 1.64	174	121, 114			
R-Ser	1	1.00, 1.00	1.71, 1.89	1.63, 1.65	176, 169	120, 112	1.68	-	1.66
	2	1.00, 1.00	1.66, 1.87	1.63, 1.64	171, 171	121, 113			
	3	1.00, 1.01	1.71	1.63, 1.63	176	123, 125	1.87	-	1.69
	4	1.00, 1.00	1.67	1.64, 1.64	177	120, 113			
S-Ser	1	1.00, 1.00	1.76, 1.89	1.63, 1.65	173, 169	122, 113	1.72	-	1.64
	2	1.00, 1.00	1.65, 1.87	1.64, 1.65	175, 170	120, 113			
	3	1.00, 0.99	1.71	1.63, 1.63	178	124, 127	1.72	-	1.73
	4	1.00, 1.01	1.68	1.64, 1.64	178	120, 114			
R-Cys¹	1	1.01, 0.99	1.82, 1.93	1.64, 1.65	175, 172	116, 112	1.75	1.54	-
	2	0.99, 1.00	1.62, 1.80	1.62, 1.65	171, 172	121, 113			
	3	1.00, 1.07	1.71	1.64, 1.62	177	121, 125	1.82	2.06	-
	4	1.01, 0.99	1.62	1.63, 1.65	174	121, 114			
S-Cys¹	1	0.99, 0.99	1.83, 1.93	1.62, 1.65	167, 166	119, 111	1.82	1.59	-
	2	0.99, 1.00	1.74, 1.84	1.65, 1.64	176, 170	118, 112			
	3	1.00, 0.99	1.68	1.63, 1.63	178	123, 125	1.72	2.28	-
	4	1.00, 1.05	1.72	1.64, 1.63	174	120, 113			
R-Cys²	1	0.99, 0.99	1.82, 1.92	1.62, 1.65	166, 167	119, 111	1.87	1.60	-
	2	0.99, 1.00	1.74, 1.88	1.64, 1.64	176, 170	118, 113			
	3	1.00, 0.99	1.70	1.63, 1.64	177	121, 126	1.76	2.16	-
	4	1.00, 1.05	1.73	1.64, 1.63	175	119, 113			
S-Cys²	1	1.01, 0.99	1.81, 1.92	1.63, 1.65	173, 168	116, 112	1.75	1.63	-
	2	0.99, 1.00	1.61, 1.81	1.62, 1.65	173, 172	121, 113			
	3	1.00, 1.04	1.72	1.64, 1.62	178	121, 127	1.85	2.14	-
	4	1.01, 0.99	1.65	1.63, 1.64	174	120, 115			

Table S.1: Selected bond lengths or angles of the DFT-optimized geometries of adsorbed amino acids on hydroxylated α -quartz (0001). Structural information for the bare surface is also included. Two different configurations with almost equal energies for each *R*- and *S*-cysteine are marked as superscript 1 and 2.