Supporting Information: Cysteine on TiO_2(110): a theoretical study by reactive dynamics and photoemission spectra simulation.

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Table S1: N1s, O1s and S2p computed binding energies (eV) of different species of cysteine in different absorption geometries (see Figs. 4-7,S1) selected by reactive dynamics.

Contacts	Adsorbate	Species	Surface	N1s	O(-H) 1s	O(=C) 1s	S2p
1	Ne-S_d-37	A_S	Defect	401.634	-	-	-
1	Z_S-S_p-02	A_S	Perfect	402.663	-	-	-
1	Z_O-S_d-16	Ne	Defect	403.166	-	-	-
1	Z_O-S_d-25	Ne	Defect	403.234	-	-	-
1	Ne-S_d-24	Ne	Defect	403.483	-	-	-
1	Z_O-S_p-16	Ne	Perfect	403.552	-	-	-
1	Z_O-S_p-35	Ne	Perfect	402.700	-	-	-
1	Ne-S_p-13	Ne	Perfect	402.396	-	-	-
1	Ne-S_d-04	Ne	Perfect	403.738	-	-	-
1	Z_O-S_d-03	A_S	Defect	-	531.336	531.100	-
1	Z_O-S_d-11	Ne	Perfect	-	537.800	535.458	-
1	Z_O-S_p-41	Ne	Perfect	-	536.843	535.778	-
1	Z_O-S_d-24	Ne	Perfect	-	537.363	535.538	-
1	Ne-S_p-04	Ne	Perfect	-	537.156	536.153	-
1	Ne-S_p-38	Ne	Perfect	-	531.778	530.667	-
1	Z_O-S_p-37	A_S	Perfect	-	-	-	165.075
1	Ne-S_p-51	A_S	Perfect	-	-	-	163.964
1	Z_O-S_d-09	Ne	Perfect	-	-	-	168.647
2	Z_S-S_p-05	A_S	Perfect	402.663	535.764	535.390	-
2	Ne-S_d-13	A_O	Defect	400.952	531.719	531.808	-
2	Ne-S_d-25	A_O	Defect	401.734	531.303	532.535	-
2	Ne-S_d-47	A_S	Perfect	400.595	536.949	535.064	-
2	Z_O-S_p-25	Ne	Perfect	403.461	536.997	535.097	-
2	Z_O-S_d-21	Ne	Perfect	404.013	537.193	535.414	-
2	Z_O-S_d-51	Ne	Perfect	402.572	536.781	535.535	-
2	Z_S-S_p-50	A_S	Perfect	403.384	-	-	164.678
2	Ne-S_p-07	A_S	Perfect	402.118	-	-	164.728
2	Ne-S_p-11	A_S	Perfect	401.492	-	-	164.186
2	Ne-S_p-16	A_S	Perfect	402.013	-	-	164.986
2	Z_O-S_d-47	A_S	Perfect	403.545	-	-	164.667
2	Z_O-S_d-18	Ne	Defect	403.154	-	-	167.637
2	Ne-S_d-23	Ne	Defect	403.856	-	-	167.739
2	Ne-S_d-27	Ne	Perfect	403.274	-	-	168.143
2	Z_S-S_p-26	A_S	Perfect	403.439	-	-	-
2	Z_O-S_p-51	A_S	Perfect	-	536.985	535.874	163.357
2	Ne-S_p-03	Ne	Perfect	-	531.105	531.779	167.112
2	Z_S-S_p-27	Z_S	Perfect	-	538.871	536.083	163.305
3	Z_O-S_d-41	A_O	Defect	402.591	534.392	534.212	168.109
3	Z_O-S_p-07	A_S	Perfect	404.086	534.777	-	-
3	Z_S-S_p-29	A_S	Perfect	403.064	536.348	535.366	-
3	Z_S-S_p-42	A_S	Perfect	-	535.943	534.785	164.275
3	Ne-S_d-41	A_S	Defect	402.246	538.201	535.672	164.176
3	Ne-S_d-49	A_S	Perfect	402.449	538.322	536.458	165.913
3	Z_S-S_d-17	Z_S	Perfect	410.535	538.049	537.005	166.041
3	Z_S-S_d-31	Z_S	Perfect	405.048	539.254	537.545	167.079

Table S2: N1s, O1s and S2p computed binding energies (eV) of different species of cysteine adsorbed on surface defects (see Fig. 11).

Contacts	Adsorbate	Species	Surface	N1s	O(-H) 1s	O(=C) 1s	S2p
2	s1	A_S	Defect	-	-	-	166.085
3	s2	A-A	Defect	-	536.559	535.487	164.611
1	s3	A_S	Defect	-	-	-	167.009
2	s4	A-A	Defect	-	-	-	166.116

Table S3: N1s, O1s and S2p computed binding energies (eV) of different species of cysteine in gas phase.

Species	N1s	O(-H) 1s	O(=C) 1s	S2p
A_O	401.061	530.727	530.686	166.170
A_S	401.319	534.197	533.167	162.458
Ne	405.434	540.033	537.902	169.849
Z_O	409.543	535.832	535.716	170.548
Z_S	409.542	539.045	537.880	167.413

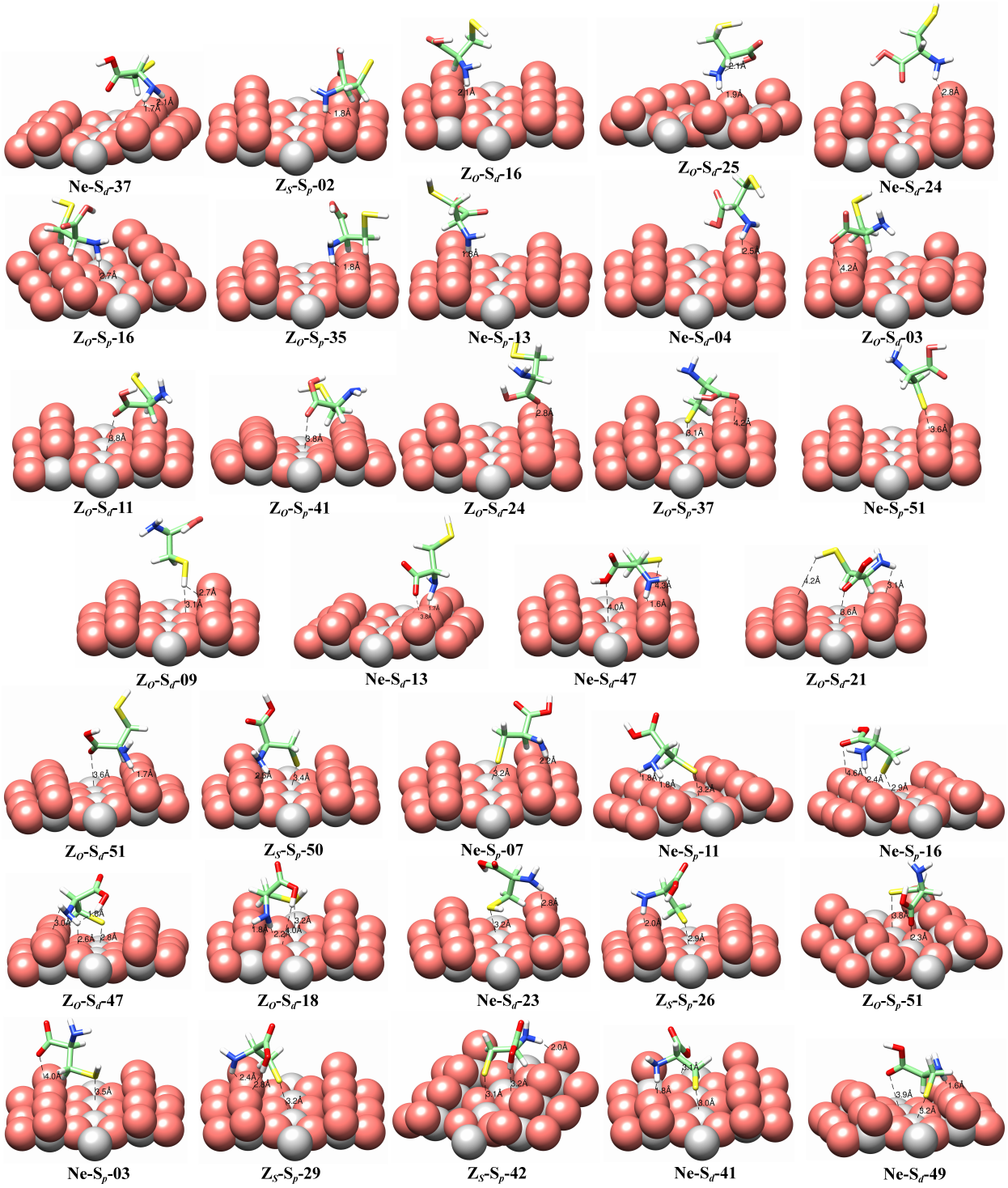

Figure S1: Other structures used in Table S1.