Appendix A electronic version

For

Modelling the interactions of engineered nanoparticles with natural organic matter using *in silico* techniques

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Table A.1: Different configurations of Ag (111) surface when the formic acid (FA1) attached.

Structures	TE	Ads	RAE	DE	FA1 : dEad/dNi
Ag (1 1 1) - FA	-36.51065712	-15.66241466	-14.96212728	-0.70028738	-15.66241466

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Formic acid(FA2)

Table A.2: Different configurations of Ag (111) surface when the acetic acid (AA1) attached.

Structures	TE	Ads	RAE	DE	AA1 : dEad/dNi
Ag (1 1 1) - AA1	-66.58111487	-21.75885732	-20.69373665	-1.06512067	-21.75885732

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Acetic acid (AA1)

Table A.3: Different configurations of Ag (111) surface when the ascorbic acid (AA2) attached.

Structures	TE	Ads	RAE	DE	AA2 : dEad/dNi
Ag (1 1 1) - AA2 - 1	-30.92835639	-69.56749644	-52.72580615	-16.8416903	-69.56749644
Ag (1 1 1) - AA2 - 2	-29.71113474	-68.3502748	-50.98543449	-17.36484031	-68.3502748

Ag (1 1 1) - AA2 - 3	-28.90593146	-67.54507152	-53.12121462	-14.4238569	-67.54507152
Ag (1 1 1) - AA2 - 4	-28.22842513	-66.86756518	-52.63108961	-14.23647557	-66.86756518
Ag (1 1 1) - AA2 - 5	-27.71112826	-66.35026832	-50.22504463	-16.12522369	-66.35026832
Ag (1 1 1) - AA2 - 6	-27.12512961	-65.76426967	-52.28601924	-13.47825042	-65.76426967
Ag (1 1 1) - AA2 - 7	-26.8409285	-65.48006856	-47.21185318	-18.26821538	-65.48006856
Ag (1 1 1) - AA2 - 8	-25.72204061	-64.36118066	-48.51110938	-15.85007128	-64.36118066
Ag (1 1 1) - AA2 - 9	-25.15092031	-63.79006037	-48.31141508	-15.47864528	-63.79006037
Ag (1 1 1) - AA2 - 10	-22.76485026	-61.40399032	-43.31471353	-18.08927679	-61.40399032
Ag (1 1 1) - AA2 - 11	-22.56469285	-61.20383291	-43.16749363	-18.03633927	-61.20383291

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Ascorbic acid(AA2)

Table A.4: Different configurations of Ag tetrahedron when the adsorbate (Formic acid 1) attached on the vertices position.

Structures	TE	Ads	RAE	DE	FA1: dEad/dNi
Ag tetrahedron + FA1 verta - 1	-33.18440817	-12.33616571	-11.6314671	-0.70469861	-12.33616571
Ag tetrahedron + FA1 verta - 2	-32.84959312	-12.00135066	-11.29758928	-0.70376138	-12.00135066
Ag tetrahedron + FA1 verta - 3	-32.5750962	-11.72685373	-11.02091117	-0.70594257	-11.72685373
Ag tetrahedron + FA1 verta - 4	-32.27667152	-11.42842905	-10.72249196	-0.70593709	-11.42842905
Ag tetrahedron + FA1 verta - 5	-32.05781014	-11.20956768	-10.50643884	-0.70312883	-11.20956768
Ag tetrahedron + FA1 verta - 6	-31.841163	-10.99292054	-10.28862988	-0.70429066	-10.99292054

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Formic acid (FA1)

Table A.5: Different configurations of Ag tetrahedron when the adsorbate (Formic acid 1) attached on the vertices position.

Structures	TE	Ads	RAE	DE	FA1 : dEad/dNi
Ag tetrahedron + FA1 vertb - 1	-40.32705425	-19.47881179	-18.77152442	-0.70728737	-19.47881179
Ag tetrahedron + FA1 vertb - 2	-40.04991527	-19.20167281	-18.49495966	-0.70671315	-19.20167281
Ag tetrahedron + FA1 vertb - 3	-39.83213856	-18.9838961	-18.28160834	-0.70228776	-18.9838961
Ag tetrahedron + FA1 vertb - 4	-39.12786046	-18.279618	-17.5730585	-0.7065595	-18.279618
Ag tetrahedron + FA1 vertb - 5	-38.75281006	-17.9045676	-17.20220886	-0.70235873	-17.9045676
Ag tetrahedron + FA1 vertb - 6	-38.43199097	-17.5837485	-16.8818619	-0.70188661	-17.5837485
Ag tetrahedron + FA1 vertb - 7	-35.60144629	-14.75320383	-14.05110347	-0.70210036	-14.75320383
Ag tetrahedron + FA1 vertb - 8	-35.33456365	-14.48632119	-13.78378045	-0.70254074	-14.48632119
Ag tetrahedron + FA1 vertb - 9	-35.08700257	-14.23876011	-13.5365561	-0.70220401	-14.23876011
Ag tetrahedron + FA1 vertb - 10	-34.62205988	-13.77381742	-13.07096265	-0.70285477	-13.77381742
Ag tetrahedron + FA1 vertb - 11	-34.40697036	-13.5587279	-12.85647189	-0.70225601	-13.5587279
Ag tetrahedron + FA1 vertb - 12	-33.97451464	-13.12627218	-12.42248603	-0.70378615	-13.12627218
Ag tetrahedron + FA1 vertb - 13	-33.73107476	-12.8828323	-12.17851402	-0.70431828	-12.8828323
Ag tetrahedron + FA1 vertb - 14	-33.35719603	-12.50895357	-11.80644748	-0.70250609	-12.50895357
Ag tetrahedron + FA1 vertb - 15	-33.13501576	-12.28677329	-11.58410426	-0.70266904	-12.28677329

Ag tetrahedron + FA1 vertb - 16	-32.35667678	-11.50843432	-10.80170841	-0.70672591	-11.50843432
Ag tetrahedron + FA1 vertb - 17	-31.95488727	-11.1066448	-10.39787347	-0.70877133	-11.1066448
Ag tetrahedron + FA1 vertb - 18	-31.67104365	-10.82280119	-10.11440156	-0.70839963	-10.82280119

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Formic acid (FA1)

Table A.6: Different configurations of Ag tetrahedron when the adsorbate (Formic acid 1) attached on the vertices position.

Structures	TE	Ads	RAE	DE	FA1 : dEad/dNi
Ag tetrahedron + FA1 vertc - 1	-40.32705425	-19.47881179	-18.77152366	-0.70728813	-19.47881179
Ag tetrahedron + FA1 vertc - 2	-39.95929814	-19.11105568	-18.40371991	-0.70733577	-19.11105568
Ag tetrahedron + FA1 vertc - 3	-37.8203985	-16.97215604	-16.26442582	-0.70773022	-16.97215604
Ag tetrahedron + FA1 vertc - 4	-35.54371292	-14.69547045	-13.99348607	-0.70198438	-14.69547045
Ag tetrahedron + FA1 vertc - 5	-35.13215602	-14.28391356	-13.58166184	-0.70225172	-14.28391356
Ag tetrahedron + FA1 vertc - 6	-34.92406107	-14.0758186	-13.37300171	-0.70281689	-14.0758186
Ag tetrahedron + FA1 vertc - 7	-34.63380512	-13.78556266	-13.0821518	-0.70341086	-13.78556266
Ag tetrahedron + FA1 vertc - 8	-34.32421684	-13.47597437	-12.77346346	-0.70251091	-13.47597437
Ag tetrahedron + FA1 vertc - 9	-34.10286903	-13.25462657	-12.55151839	-0.70310817	-13.25462657
Ag tetrahedron + FA1 vertc - 10	-33.87674516	-13.0285027	-12.32427481	-0.70422789	-13.0285027
Ag tetrahedron + FA1 vertc - 11	-33.63082284	-12.78258037	-12.07718716	-0.70539321	-12.78258037
Ag tetrahedron + FA1 vertc - 12	-33.41747905	-12.56923659	-11.86466906	-0.70456753	-12.56923659
Ag tetrahedron + FA1 vertc - 13	-33.1311279	-12.28288543	-11.57999212	-0.70289331	-12.28288543
Ag tetrahedron + FA1 vertc - 14	-32.80078618	-11.95254371	-11.24977468	-0.70276903	-11.95254371
Ag tetrahedron + FA1 vertc - 15	-32.35667678	-11.50843432	-10.80170885	-0.70672546	-11.50843432
Ag tetrahedron + FA1 vertc - 16	-31.95488727	-11.10664481	-10.39787336	-0.70877144	-11.10664481
Ag tetrahedron + FA1vertc - 17	-31.61974808	-10.77150561	-10.06440328	-0.70710233	-10.77150561
Ag tetrahedron + FA1vertc - 18	-30.2355953	-9.38735284	-8.67909626	-0.70825658	-9.38735284

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Former acid (FA1)

Table A.7: Different configurations of Ag tetrahedron when the adsorbate (Formic acid 1) attached on the face.

Structures	TE	Ads	RAE	DE	FA1: dEad/dNi
Ag tetrahedron + FA1 face - 1	-40.32705424	-19.47881178	-18.77152656	-0.70728521	-19.47881178
Ag tetrahedron + FA1 face - 2	-40.04991526	-19.20167279	-18.49496366	-0.70670913	-19.20167279
Ag tetrahedron + FA 1face - 3	-39.71436872	-18.86612625	-18.16290615	-0.7032201	-18.86612625
Ag tetrahedron + FA1 face - 4	-38.28978549	-17.44154303	-16.73608395	-0.70545908	-17.44154303
Ag tetrahedron + FA1 face - 5	-37.87602627	-17.0277838	-16.32318376	-0.70460005	-17.0277838
Ag tetrahedron + FA1 face - 6	-37.62778418	-16.77954171	-16.07093033	-0.70861138	-16.77954171
Ag tetrahedron + FA1 face - 7	-37.34373544	-16.49549298	-15.7881305	-0.70736248	-16.49549298
Ag tetrahedron + FA1 face - 8	-37.00908985	-16.16084739	-15.45212545	-0.70872194	-16.16084739
Ag tetrahedron + FA1 face - 9	-36.72346504	-15.87522258	-15.16879056	-0.70643202	-15.87522258
Ag tetrahedron + FA1 face - 10	-36.49837389	-15.65013143	-14.94310608	-0.70702535	-15.65013143
Ag tetrahedron + FA1 face - 11	-36.27396647	-15.425724	-14.71711065	-0.70861335	-15.425724
Ag tetrahedron + FA1 face - 12	-36.05791757	-15.20967511	-14.50400334	-0.70567176	-15.20967511
Ag tetrahedron + FA1 face - 13	-35.65332201	-14.80507954	-14.09842889	-0.70665065	-14.80507954
Ag tetrahedron + FA1 face - 14	-34.24281585	-13.39457339	-12.69156287	-0.70301052	-13.39457339
Ag tetrahedron + FA1 face - 15	-34.01902316	-13.1707807	-12.46756502	-0.70321568	-13.1707807
Ag tetrahedron + FA1 face - 16	-33.73181674	-12.88357428	-12.17848395	-0.70509032	-12.88357428
Ag tetrahedron + FA1 face - 17	-33.52274132	-12.67449886	-11.96921274	-0.70528612	-12.67449886
Ag tetrahedron + FA1 face - 18	-33.28609166	-12.4378492	-11.732747	-0.7051022	-12.4378492
Ag tetrahedron + FA1 face - 19	-33.05048704	-12.20224457	-11.49931433	-0.70293025	-12.20224457
Ag tetrahedron + FA1 face - 20	-32.84959312	-12.00135066	-11.29758515	-0.7037655	-12.00135066
Ag tetrahedron + FA1 face - 21	-31.83294689	-10.98470443	-10.28164347	-0.70306096	-10.98470443

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Formic acid (FA1)

Table A.8: Different configurations of Ag tetrahedron when the adsorbate (Formic acid 1) attached on the edge.

Structures	TE	Ads	RAE	DE	FA1 : dEad/dNi
Ag tetrahedron + FA1 edge - 1	-40.04991527	-19.20167281	-18.49496164	-0.70671116	-19.20167281
Ag tetrahedron + FA1 edge - 2	-39.42794036	-18.5796979	-17.87131461	-0.70838329	-18.5796979
Ag tetrahedron + FA1 edge - 3	-35.53384156	-14.68559909	-13.98343738	-0.70216172	-14.68559909
Ag tetrahedron + FA1 edge - 4	-35.20372614	-14.35548368	-13.65265584	-0.70282783	-14.35548368
Ag tetrahedron + FA1 edge - 5	-34.96188942	-14.11364696	-13.41144685	-0.7022001	-14.11364696
Ag tetrahedron + FA1 edge - 6	-34.63380512	-13.78556266	-13.08215238	-0.70341028	-13.78556266
Ag tetrahedron + FA1 edge - 7	-34.32421685	-13.47597438	-12.7734672	-0.70250718	-13.47597438
Ag tetrahedron + FA1 edge - 8	-34.10286903	-13.25462657	-12.55151762	-0.70310894	-13.25462657
Ag tetrahedron + FA1 edge - 9	-33.87674516	-13.02850269	-12.32427342	-0.70422928	-13.02850269
Ag tetrahedron + FA1 edge - 10	-33.63418994	-12.78594748	-12.08058569	-0.70536179	-12.78594748
Ag tetrahedron + FA1 edge - 11	-33.35719601	-12.50895355	-11.80644852	-0.70250503	-12.50895355
Ag tetrahedron + FA1 edge - 12	-33.13501576	-12.28677329	-11.58410649	-0.7026668	-12.28677329
Ag tetrahedron + FA1 edge - 13	-32.72366535	-11.87542288	-11.16962977	-0.70579312	-11.87542288
Ag tetrahedron + FA1 edge - 14	-32.35667678	-11.50843432	-10.80171051	-0.70672381	-11.50843432
Ag tetrahedron + FA1 edge - 15	-31.95488727	-11.1066448	-10.39787326	-0.70877154	-11.1066448
Ag tetrahedron + FA1 edge - 16	-31.61974808	-10.77150561	-10.06440225	-0.70710337	-10.77150561

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Formic acid (FA1)

Table A.9: Different configurations of Ag tetrahedron when the (AA1) attached on the vertices position.

Structures	TE	Ads	RAE	DE	AA1: dEad/dNi
Ag tetrahedron + AA1 verta – 1	-61.71695368	-16.89469613	-15.79054239	-1.10415374	-16.89469613
Ag tetrahedron + AA1 verta – 2	-61.49981131	-16.67755376	-15.56514562	-1.11240814	-16.67755376
Ag tetrahedron + AA1 verta – 3	-61.24436891	-16.42211136	-15.3747664	-1.04734496	-16.42211136
Ag tetrahedron + AA1 verta – 4	-60.99739553	-16.17513798	-15.10143573	-1.07370225	-16.17513798
Ag tetrahedron + AA1 verta – 5	-60.71954331	-15.89728576	-14.79111895	-1.1061668	-15.89728576
Ag tetrahedron + AA1 verta - 6	-60.40349874	-15.58124119	-14.42095508	-1.16028611	-15.58124119
Ag tetrahedron + AA1 verta - 7	-59.73054393	-14.90828638	-13.71175527	-1.19653112	-14.90828638
Ag tetrahedron + AA1 verta - 8	-56.46787911	-11.64562156	-10.42101999	-1.22460157	-11.64562156

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Acetic acid (AA1)

Table A.10: Different configurations of Ag tetrahedron when the acetic acid (AA1) attached on the vertices position.

Structures	TE	Ads	RAE	DE	AA1: dEad/dNi
Ag tetrahedron + AA1 vertb - 1	-70.93545812	-26.11320057	-25.17158986	-0.94161071	-26.11320057
Ag tetrahedron + AA1 vertb - 2	-70.61508321	-25.79282566	-24.6011952	-1.19163046	-25.79282566
Ag tetrahedron + AA1 vertb - 3	-70.38808587	-25.56582832	-24.35473153	-1.21109678	-25.56582832
Ag tetrahedron + AA1 vertb - 4	-70.07689424	-25.25463669	-24.10426624	-1.15037044	-25.25463669
Ag tetrahedron + AA1 vertb - 5	-69.75505962	-24.93280207	-23.77833824	-1.15446383	-24.93280207
Ag tetrahedron + AA1 vertb - 6	-68.49267844	-23.67042089	-22.49873674	-1.17168415	-23.67042089
Ag tetrahedron + AA1 vertb - 7	-68.16905746	-23.34679991	-22.24387274	-1.10292716	-23.34679991
Ag tetrahedron + AA1 vertb - 8	-67.91408698	-23.09182943	-22.29865148	-0.79317795	-23.09182943
Ag tetrahedron + AA1 vertb - 9	-67.62794507	-22.80568752	-21.61949452	-1.186193	-22.80568752
Ag tetrahedron + AA1 vertb - 10	-67.27483442	-22.45257687	-21.63761609	-0.81496078	-22.45257687
Ag tetrahedron + AA1 vertb - 11	-66.44272454	-21.62046699	-20.41939865	-1.20106834	-21.62046699
Ag tetrahedron + AA1 vertb - 12	-65.25193949	-20.42968194	-19.35644791	-1.07323403	-20.42968194
Ag tetrahedron + AA1 vertb - 13	-64.99303167	-20.17077412	-19.12565035	-1.04512377	-20.17077412
Ag tetrahedron + AA1 vertb - 14	-64.65093733	-19.82867978	-18.78469417	-1.04398561	-19.82867978

Ag tetrahedron + AA1 vertb - 15	-64.41289619	-19.59063864	-18.48920936	-1.10142928	-19.59063864
Ag tetrahedron + AA1 vertb - 16	-64.02619314	-19.20393559	-18.15085473	-1.05308086	-19.20393559
Ag tetrahedron + AA1 vertb - 17	-63.80382755	-18.98157	-17.92598743	-1.05558257	-18.98157
Ag tetrahedron + AA1 vertb - 18	-63.58197777	-18.75972022	-17.61896909	-1.14075113	-18.75972022
Ag tetrahedron + AA1 vertb - 19	-63.34333707	-18.52107952	-17.47949445	-1.04158507	-18.52107952
Ag tetrahedron + AA1 vertb - 20	-62.82270287	-18.00044532	-16.94338474	-1.05706058	-18.00044532
Ag tetrahedron + AA1 vertb - 21	-62.6066075	-17.78434995	-16.69472712	-1.08962282	-17.78434995
Ag tetrahedron + AA1 vertb - 22	-62.27414378	-17.45188623	-16.27736356	-1.17452267	-17.45188623
Ag tetrahedron + AA1 vertb - 23	-62.0334665	-17.21120895	-16.28802727	-0.92318167	-17.21120895
Ag tetrahedron + AA1 vertb - 24	-61.82434913	-17.00209158	-16.09088632	-0.91120526	-17.00209158
Ag tetrahedron + AA1 vertb - 25	-60.81343411	-15.99117656	-14.95478641	-1.03639015	-15.99117656
Ag tetrahedron + AA1 vertb - 26	-59.17718125	-14.3549237	-13.18118721	-1.17373649	-14.3549237
Ag tetrahedron + AA1 vertb - 27	-58.81318869	-13.99093114	-12.76779879	-1.22313235	-13.99093114
Ag tetrahedron + AA1 vertb - 28	-58.53363939	-13.71138184	-12.78260623	-0.92877561	-13.71138184
Ag tetrahedron + AA1 vertb - 30	-58.26265515	-13.4403976	-12.22680281	-1.2135948	-13.4403976
Ag tetrahedron + AA1 vertb - 32	-57.89008624	-13.06782869	-11.84858944	-1.21923926	-13.06782869

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Acetic acid (AA1)

Table A.11: Different configurations of Ag tetrahedron when the acetic acid (AA1) attached on the vertices position.

Structures	TE	Ads	RAS	DE	AA1 : dEad/dNi
Ag tetrahedron + AA1 vertc - 1	-65.22006851	-20.39781096	-19.32301408	-1.07479688	-20.39781096
Ag tetrahedron + AA1 vertc - 2	-64.79852514	-19.97626759	-18.87885329	-1.09741431	-19.97626759
Ag tetrahedron + AA1 vertc - 3	-64.58170517	-19.75944762	-18.69028321	-1.06916441	-19.75944762
Ag tetrahedron + AA1 vertc - 4	-64.37625478	-19.55399723	-18.51168517	-1.04231206	-19.55399723
Ag tetrahedron + AA1 vertc - 5	-64.02619317	-19.20393562	-18.15085109	-1.05308454	-19.20393562
Ag tetrahedron + AA1 vertc - 6	-63.80382749	-18.98156994	-17.92591158	-1.05565835	-18.98156994
Ag tetrahedron + AA1 vertc - 7	-63.58197775	-18.7597202	-17.61897784	-1.14074235	-18.7597202
Ag tetrahedron + AA1 vertc - 8	-63.10834045	-18.2860829	-17.16387774	-1.12220517	-18.2860829
Ag tetrahedron + AA1 vertc - 9	-62.88314984	-18.06089229	-16.9148672	-1.14602509	-18.06089229
Ag tetrahedron + AA1 vertc - 10	-62.61388	-17.79162245	-16.76600122	-1.02562123	-17.79162245
Ag tetrahedron + AA1 vertc - 11	-62.27414381	-17.45188626	-16.27738724	-1.17449902	-17.45188626
Ag tetrahedron + AA1 vertc - 12	-62.0334665	-17.21120895	-16.28800719	-0.92320175	-17.21120895
Ag tetrahedron + AA1 vertc - 13	-61.82434913	-17.00209158	-16.09087825	-0.91121333	-17.00209158
Ag tetrahedron + AA1 vertc - 14	-61.50107463	-16.67881708	-15.4897063	-1.18911078	-16.67881708
Ag tetrahedron + AA1 vertc - 15	-61.0570187	-16.23476114	-15.28364946	-0.95111168	-16.23476114
Ag tetrahedron + AA1 vertc - 16	-60.71340135	-15.89114379	-14.86590759	-1.02523621	-15.89114379
Ag tetrahedron + AA1 vertc - 17	-59.17718114	-14.35492359	-13.181139	-1.17378459	-14.35492359
Ag tetrahedron + AA1 vertc - 18	-58.8131887	-13.99093115	-12.76779683	-1.22313433	-13.99093115
Ag tetrahedron + AA1 vertc - 19	-58.49259197	-13.67033442	-12.72811628	-0.94221813	-13.67033442
Ag tetrahedron + AA1 vertc - 20	-58.26265512	-13.44039757	-12.22680206	-1.21359551	-13.44039757
Ag tetrahedron + AA1 vertc - 21	-57.86423399	-13.04197644	-11.8227894	-1.21918704	-13.04197644
Ag tetrahedron + AA1 vertc - 22	-57.63980216	-12.81754461	-11.61212435	-1.20542026	-12.81754461
Ag tetrahedron + AA1 vertc - 23	-57.20708174	-12.38482419	-11.19100661	-1.19381758	-12.38482419

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Acetic acid (AA1)

Table A.12: Different configurations of Ag tetrahedron when the acetic acid (AA1) attached on the face.

Structures	TE	Ads	RAE	DE	AA1 : dEad/dNi
Ag tetrahedron + AA1 face - 1	-70.61508321	-25.79282566	-24.60118653	-1.19163913	-25.79282566
Ag tetrahedron + AA1 face - 2	-66.9439778	-22.12172024	-21.35215344	-0.7695668	-22.12172024
Ag tetrahedron + AA1 face - 3	-66.64211225	-21.81985469	-21.05562015	-0.76423455	-21.81985469
Ag tetrahedron + AA1 face - 4	-66.11033878	-21.28808122	-20.08173457	-1.20634666	-21.28808122
Ag tetrahedron + AA1 face - 5	-65.81603363	-20.99377608	-19.79138056	-1.20239552	-20.99377608
Ag tetrahedron + AA1 face - 6	-65.54841835	-20.7261608	-19.78254542	-0.94361538	-20.7261608
Ag tetrahedron + AA1 face - 7	-65.2997301	-20.47747255	-19.73081968	-0.74665287	-20.47747255
Ag tetrahedron + AA1 face - 8	-64.99092026	-20.16866271	-19.14592731	-1.02273541	-20.16866271
Ag tetrahedron + AA1 face - 9	-64.70733507	-19.88507752	-18.6740682	-1.21100932	-19.88507752
Ag tetrahedron + AA1 face - 10	-64.37500455	-19.552747	-18.40424377	-1.14850323	-19.552747
Ag tetrahedron + AA1 face - 11	-64.1660428	-19.34378525	-18.54835729	-0.79542796	-19.34378525
Ag tetrahedron + AA1 face - 12	-63.19234206	-18.37008451	-17.29547917	-1.07460535	-18.37008451
Ag tetrahedron + AA1 face - 13	-62.94722564	-18.12496809	-17.07843576	-1.04653233	-18.12496809
Ag tetrahedron + AA1 face - 14	-62.55766405	-17.7354065	-16.74012644	-0.99528006	-17.7354065
Ag tetrahedron + AA1 face - 15	-62.34353953	-17.52128198	-16.38172716	-1.13955482	-17.52128198
Ag tetrahedron + AA1 face - 16	-62.12767759	-17.30542004	-16.21057752	-1.09484252	-17.30542004
Ag tetrahedron + AA1 face - 17	-61.77523511	-16.95297756	-15.84649258	-1.10648498	-16.95297756
Ag tetrahedron + AA1 face - 18	-61.54584805	-16.7235905	-15.62606503	-1.09752547	-16.7235905
Ag tetrahedron + AA1 face - 19	-61.29889538	-16.47663783	-15.41534095	-1.06129688	-16.47663783
Ag tetrahedron + AA1 face - 20	-61.08110459	-16.25884704	-15.05188924	-1.2069578	-16.25884704
Ag tetrahedron + AA1 face - 21	-55.35862537	-10.53636782	-9.3190947	-1.21727312	-10.53636782

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Acetic acid (AA1)

Table A.13: Different configurations of Ag tetrahedron when the acetic acid (AA1) attached on the edge.

Structures	TE	Ads	RAE	DE	AA1: dEad/dNi
Ag tetrahedron + AA1 edge - 1	-65.2200684	-20.39781085	-19.32288895	-1.0749219	-20.39781085
Ag tetrahedron + AA1 edge - 2	-64.80754649	-19.98528894	-18.93429318	-1.05099576	-19.98528894
Ag tetrahedron + AA1 edge - 3	-64.60193947	-19.77968192	-18.66288369	-1.11679823	-19.77968192
Ag tetrahedron + AA1 edge - 4	-64.37625476	-19.55399721	-18.51172364	-1.04227357	-19.55399721
Ag tetrahedron + AA1 edge - 5	-63.83969364	-19.01743609	-17.9570208	-1.06041529	-19.01743609
Ag tetrahedron + AA1 edge - 6	-63.59482293	-18.77256538	-17.69367575	-1.07888963	-18.77256538
Ag tetrahedron + AA1 edge - 7	-63.34333708	-18.52107953	-17.47952884	-1.04155069	-18.52107953
Ag tetrahedron + AA1 edge - 8	-63.05355484	-18.23129729	-17.1691914	-1.06210589	-18.23129729
Ag tetrahedron + AA1 edge - 9	-62.83421872	-18.01196117	-16.86390138	-1.14805979	-18.01196117
Ag tetrahedron + AA1 edge - 10	-62.61388	-17.79162245	-16.76601312	-1.02560933	-17.79162245
Ag tetrahedron + AA1 edge - 11	-62.27414382	-17.45188627	-16.27738587	-1.1745004	-17.45188627
Ag tetrahedron + AA1 edge - 12	-62.0334665	-17.21120895	-16.28802964	-0.92317931	-17.21120895
Ag tetrahedron + AA1 edge - 13	-61.82434912	-17.00209157	-16.09088839	-0.91120319	-17.00209157
Ag tetrahedron + AA1 edge - 14	-61.50107463	-16.67881708	-15.48970563	-1.18911145	-16.67881708
Ag tetrahedron + AA1 edge - 15	-61.05701869	-16.23476114	-15.28366817	-0.95109297	-16.23476114
Ag tetrahedron + AA1 edge - 16	-60.81343411	-15.99117656	-14.95479655	-1.03638001	-15.99117656
Ag tetrahedron + AA1 edge - 17	-59.54776946	-14.72551191	-13.67719685	-1.04831505	-14.72551191
Ag tetrahedron + AA1 edge - 18	-59.17718119	-14.35492364	-13.18120194	-1.1737217	-14.35492364
Ag tetrahedron + AA1 edge - 19	-58.8131887	-13.99093115	-12.7677947	-1.22313645	-13.99093115
Ag tetrahedron + AA1 edge - 20	-58.53363939	-13.71138184	-12.78258596	-0.92879587	-13.71138184
Ag tetrahedron + AA1 edge - 21	-58.23411411	-13.41185656	-12.19827145	-1.21358511	-13.41185656
Ag tetrahedron + AA1 edge - 22	-57.864234	-13.04197644	-11.82278678	-1.21918967	-13.04197644
Ag tetrahedron + AA1 edge - 23	-57.6223395	-12.80008195	-11.67366121	-1.12642073	-12.80008195
Ag tetrahedron + AA1 edge - 24	-57.20708174	-12.38482419	-11.19099741	-1.19382678	-12.38482419

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Acetic acid (AA1)

Table A.14: Different configurations of Ag tetrahedron when the acetic acid (AA2) attached on the vertices position.

Structures	TE	Ads	RAE	DE	AA2: dEad/dNi
Ag tetrahedron + AA2 verta - 1	-16.61241752	-55.25155757	-35.03280402	-20.21875356	-55.25155757
Ag tetrahedron + AA2 verta - 2	-16.09412294	-54.733263	-36.58405206	-18.14921094	-54.733263
Ag tetrahedron + AA2 verta - 3	-15.50757028	-54.14671034	-36.12734876	-18.01936158	-54.14671034
Ag tetrahedron + AA2 verta - 4	-15.09834982	-53.73748988	-34.96912984	-18.76836004	-53.73748988
Ag tetrahedron + AA2 verta - 5	-13.81967165	-52.4588117	-32.78611188	-19.67269982	-52.4588117
Ag tetrahedron + AA2 verta - 6	-10.83239681	-49.47153687	-30.53896354	-18.93257332	-49.47153687
Ag tetrahedron + AA2 verta - 7	-10.57493014	-49.21407019	-29.84685999	-19.36721021	-49.21407019
Ag tetrahedron + AA2 verta - 8	-10.3392452	-48.97838525	-30.0080989	-18.97028636	-48.97838525
Ag tetrahedron + AA2 verta - 9	-9.91632946	-48.55546951	-30.01080122	-18.5446683	-48.55546951
Ag tetrahedron + AA2 verta - 10	-8.49971831	-47.13885837	-28.04086973	-19.09798864	-47.13885837
Ag tetrahedron + AA2 verta - 11	-8.25458943	-46.89372949	-29.05735861	-17.83637088	-46.89372949
Ag tetrahedron + AA2 verta - 12	-7.90111322	-46.54025328	-27.64259834	-18.89765494	-46.54025328
Ag tetrahedron + AA2 verta - 13	-7.45111613	-46.09025619	-27.15552682	-18.93472937	-46.09025619
Ag tetrahedron + AA2 verta - 14	-7.16089432	-45.80003438	-27.76337346	-18.03666092	-45.80003438
Ag tetrahedron + AA2 verta - 15	-6.95213646	-45.59127651	-27.46462441	-18.1266521	-45.59127651
Ag tetrahedron + AA2 verta - 16	-6.64713484	-45.2862749	-25.16760163	-20.11867326	-45.2862749
Ag tetrahedron + AA2 verta - 17	-6.10872892	-44.74786898	-26.29010131	-18.45776767	-44.74786898
Ag tetrahedron + AA2 verta - 18	-5.8828074	-44.52194746	-25.9993068	-18.52264066	-44.52194746
Ag tetrahedron + AA2 verta - 19	-5.47355349	-44.11269355	-26.03083443	-18.08185913	-44.11269355
Ag tetrahedron + AA2 verta - 20	-4.94027894	-43.579419	-24.80315491	-18.77626409	-43.579419
Ag tetrahedron + AA2 verta - 21	-4.39531556	-43.03445562	-24.12878393	-18.90567169	-43.03445562
Ag tetrahedron + AA2 verta - 22	-4.03850822	-42.67764828	-24.10032441	-18.57732386	-42.67764828
Ag tetrahedron + AA2 verta - 23	-3.83150122	-42.47064128	-24.3303809	-18.14026038	-42.47064128
Ag tetrahedron + AA2 verta - 24	-3.6209242	-42.26006426	-23.97625097	-18.28381329	-42.26006426
Ag tetrahedron + AA2 verta - 25	-3.12583064	-41.7649707	-22.67670883	-19.08826187	-41.7649707
Ag tetrahedron + AA2 verta - 26	-2.88125623	-41.52039629	-22.9914474	-18.52894889	-41.52039629

Ag tetrahedron + AA2 verta - 27	-2.66082987	-41.29996993	-22.78641519	-18.51355474	-41.29996993
Ag tetrahedron + AA2 verta - 28	-2.16194649	-40.80108655	-22.44880566	-18.35228089	-40.80108655
Ag tetrahedron + AA2 verta - 29	-1.80209107	-40.44123112	-21.35479914	-19.08643199	-40.44123112
Ag tetrahedron + AA2 verta - 30	-1.5239679	-40.16310796	-20.91070252	-19.25240543	-40.16310796
Ag tetrahedron + AA2 verta - 31	-1.26554644	-39.9046865	-21.50713844	-18.39754806	-39.9046865
Ag tetrahedron + AA2 verta - 32	-0.45698591	-39.09612597	-19.4907936	-19.60533237	-39.09612597
Ag tetrahedron + AA2 verta - 33	-0.08413538	-38.72327544	-20.19084657	-18.53242887	-38.72327544
Ag tetrahedron + AA2 verta - 34	0.14483655	-38.49430351	-19.65095973	-18.84334377	-38.49430351
Ag tetrahedron + AA2 verta - 35	0.74713663	-37.89200343	-18.96973237	-18.92227105	-37.89200343

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Ascorbic acid (AA2)

Table A.15: Different configurations of Ag tetrahedron when the acetic acid (AA2) attached on the vertices position.

Structures	TE	Ads	RAE	DE	AA2: dEad/dNi
Ag tetrahedron + AA2 vertb - 1	-27.45358021	-66.09272027	-46.45028727	-19.642433	-66.09272027
Ag tetrahedron + AA2 vertb - 2	-26.72473562	-65.36387568	-46.35171225	-19.01216343	-65.36387568
Ag tetrahedron + AA2 vertb - 3	-25.1271186	-63.76625866	-44.4364653	-19.32979336	-63.76625866
Ag tetrahedron + AA2 vertb - 4	-24.55576728	-63.19490733	-45.04003181	-18.15487552	-63.19490733
Ag tetrahedron + AA2 vertb - 5	-23.98741289	-62.62655295	-42.88082939	-19.74572356	-62.62655295
Ag tetrahedron + AA2 vertb - 6	-23.61028382	-62.24942388	-42.61908156	-19.63034232	-62.24942388
Ag tetrahedron + AA2 vertb - 7	-23.27246216	-61.91160221	-43.04569998	-18.86590223	-61.91160221
Ag tetrahedron + AA2 vertb - 8	-23.06287033	-61.70201039	-42.51098106	-19.19102933	-61.70201039
Ag tetrahedron + AA2 vertb - 9	-22.83817813	-61.47731818	-43.37346978	-18.1038484	-61.47731818
Ag tetrahedron + AA2 vertb - 10	-22.53670373	-61.17584378	-42.90535621	-18.27048758	-61.17584378
Ag tetrahedron + AA2 vertb - 11	-22.27369891	-60.91283897	-40.98948859	-19.92335038	-60.91283897
Ag tetrahedron + AA2 vertb - 12	-21.96210182	-60.60124188	-43.14949335	-17.45174853	-60.60124188
Ag tetrahedron + AA2 vertb - 13	-21.65885395	-60.297994	-41.39560209	-18.90239191	-60.297994
Ag tetrahedron + AA2 vertb - 14	-21.0105654	-59.64970546	-40.62319553	-19.02650992	-59.64970546
Ag tetrahedron + AA2 vertb - 15	-20.38311528	-59.02225534	-41.82330448	-17.19895085	-59.02225534
Ag tetrahedron + AA2 vertb - 16	-20.07452944	-58.7136695	-39.32358474	-19.39008476	-58.7136695

Ag tetrahedron + AA2 vertb - 17	-19.58151753	-58.22065759	-39.80065199	-18.4200056	-58.22065759
Ag tetrahedron + AA2 vertb - 18	-19.29094185	-57.9300819	-40.32524396	-17.60483794	-57.9300819
Ag tetrahedron + AA2 vertb - 19	-18.96338793	-57.60252799	-39.73528475	-17.86724324	-57.60252799
Ag tetrahedron + AA2 vertb - 20	-18.55942326	-57.19856332	-39.26716048	-17.93140284	-57.19856332
Ag tetrahedron + AA2 vertb - 21	-18.13675207	-56.77589213	-39.48463283	-17.2912593	-56.77589213
Ag tetrahedron + AA2 vertb - 22	-17.77371641	-56.41285647	-37.5452292	-18.86762727	-56.41285647
Ag tetrahedron + AA2 vertb - 23	-17.35967267	-55.99881273	-36.91466372	-19.08414901	-55.99881273
Ag tetrahedron + AA2 vertb - 24	-17.04093548	-55.68007553	-38.39160689	-17.28846865	-55.68007553
Ag tetrahedron + AA2 vertb - 25	-16.73235787	-55.37149793	-41.77520206	-13.59629587	-55.37149793
Ag tetrahedron + AA2 vertb - 26	-16.50649109	-55.14563115	-36.23563132	-18.90999983	-55.14563115
Ag tetrahedron + AA2 vertb - 27	-16.25242383	-54.89156389	-35.01424457	-19.87731932	-54.89156389
Ag tetrahedron + AA2 vertb - 28	-16.02314877	-54.66228883	-34.95542471	-19.70686412	-54.66228883
Ag tetrahedron + AA2 vertb - 29	-15.81161465	-54.45075471	-34.82458762	-19.62616709	-54.45075471
Ag tetrahedron + AA2 vertb - 30	-15.59111167	-54.23025172	-36.06155252	-18.16869921	-54.23025172
Ag tetrahedron + AA2 vertb - 31	-15.35367867	-53.99281873	-34.87128306	-19.12153567	-53.99281873
Ag tetrahedron + AA2 vertb - 32	-15.11327701	-53.75241707	-33.9963161	-19.75610097	-53.75241707
Ag tetrahedron + AA2 vertb - 33	-14.83952676	-53.47866682	-34.76927806	-18.70938876	-53.47866682
Ag tetrahedron + AA2 vertb - 34	-14.62997076	-53.26911081	-33.67261079	-19.59650002	-53.26911081
Ag tetrahedron + AA2 vertb - 35	-14.38832118	-53.02746123	-33.88056015	-19.14690108	-53.02746123
Ag tetrahedron + AA2 vertb - 36	-14.05773913	-52.69687919	-33.24540795	-19.45147125	-52.69687919
Ag tetrahedron + AA2 vertb - 37	-13.51767235	-52.1568124	-33.24917665	-18.90763575	-52.1568124
Ag tetrahedron + AA2 vertb - 38	-12.90788962	-51.54702968	-33.38991424	-18.15711544	-51.54702968
Ag tetrahedron + AA2 vertb - 39	-12.67120803	-51.31034808	-32.9337611	-18.37658698	-51.31034808
Ag tetrahedron + AA2 vertb - 40	-12.36883106	-51.00797111	-32.67266556	-18.33530556	-51.00797111
Ag tetrahedron + AA2 vertb - 41	-11.88742392	-50.52656398	-32.58527648	-17.9412875	-50.52656398
Ag tetrahedron + AA2 vertb - 42	-11.44657228	-50.08571234	-30.04461875	-20.04109359	-50.08571234
Ag tetrahedron + AA2 vertb - 43	-10.96066248	-49.59980254	-31.58133452	-18.01846802	-49.59980254
Ag tetrahedron + AA2 vertb - 44	-10.74595369	-49.38509375	-29.2684823	-20.11661144	-49.38509375
Ag tetrahedron + AA2 vertb - 45	-10.17154277	-48.81068283	-28.81788076	-19.99280207	-48.81068283

Ag tetrahedron + AA2 vertb - 46	-9.58806774	-48.2272078	-28.87873575	-19.34847205	-48.2272078
Ag tetrahedron + AA2 vertb - 47	-9.23769527	-47.87683532	-28.84230364	-19.03453168	-47.87683532
Ag tetrahedron + AA2 vertb - 48	-8.92006563	-47.55920568	-28.55300532	-19.00620037	-47.55920568
Ag tetrahedron + AA2 vertb - 49	-8.70076483	-47.33990489	-34.8244131	-12.51549179	-47.33990489
Ag tetrahedron + AA2 vertb - 50	-8.39087192	-47.03001198	-28.74322354	-18.28678844	-47.03001198
Ag tetrahedron + AA2 vertb - 51	-7.68597263	-46.32511269	-28.33047898	-17.99463371	-46.32511269
Ag tetrahedron + AA2 vertb - 52	-4.28105551	-42.92019557	-22.78799791	-20.13219766	-42.92019557
Ag tetrahedron + AA2 vertb - 53	-3.64773961	-42.28687967	-22.76432698	-19.52255269	-42.28687967
Ag tetrahedron + AA2 vertb - 54	-3.4420366	-42.08117666	-22.62213123	-19.45904543	-42.08117666
Ag tetrahedron + AA2 vertb - 55	-2.99750956	-41.63664961	-21.9839747	-19.65267491	-41.63664961
Ag tetrahedron + AA2 vertb - 56	-2.65687455	-41.2960146	-21.74968125	-19.54633335	-41.2960146
Ag tetrahedron + AA2 vertb - 57	-1.2148217	-39.85396175	-19.59681369	-20.25714806	-39.85396175
Ag tetrahedron + AA2 vertb - 58	-0.67960917	-39.31874923	-19.66059115	-19.65815807	-39.31874923
Ag tetrahedron + AA2 vertb - 59	-0.38019068	-39.01933074	-20.39449989	-18.62483085	-39.01933074
Ag tetrahedron + AA2 vertb - 60	-0.03536892	-38.67450898	-19.960007	-18.71450197	-38.67450898
Ag tetrahedron + AA2 vertb - 61	1.22095805	-37.41818201	-17.7151486	-19.70303341	-37.41818201
Ag tetrahedron + AA2 vertb - 62	2.26114208	-36.37799798	-16.24997823	-20.12801976	-36.37799798
Ag tetrahedron + AA2 vertb - 63	2.82899237	-35.81014768	-16.29233124	-19.51781644	-35.81014768

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Ascorbic acid (AA2)

Table A.16: Different configurations of Ag tetrahedron when the ascorbic acid (AA2) attached on the vertices position.

Structures	TE	Ads	RAE	DE	AA2: dEad/dNi
Ag tetrahedron + AA2 vertc - 1	-23.61028365	-62.2494237	-42.61906564	-19.63035807	-62.2494237
Ag tetrahedron + AA2 vertc - 2	-22.82683983	-61.46597988	-42.45283489	-19.01314499	-61.46597988
Ag tetrahedron + AA2 vertc - 3	-21.17279225	-59.8119323	-41.23438447	-18.57754783	-59.8119323
Ag tetrahedron + AA2 vertc - 4	-18.68378388	-57.32292393	-40.11060874	-17.21231519	-57.32292393
Ag tetrahedron + AA2 vertc - 5	-18.42935161	-57.06849167	-39.05786992	-18.01062175	-57.06849167
Ag tetrahedron + AA2 vertc - 6	-18.21767747	-56.85681753	-39.77986151	-17.07695602	-56.85681753
Ag tetrahedron + AA2 vertc - 7	-17.81677208	-56.45591214	-36.90909697	-19.54681516	-56.45591214
Ag tetrahedron + AA2 vertc - 8	-17.44689356	-56.08603362	-37.49990194	-18.58613169	-56.08603362
Ag tetrahedron + AA2 vertc - 9	-17.10967805	-55.74881811	-36.81257096	-18.93624715	-55.74881811
Ag tetrahedron + AA2 vertc - 10	-16.90931865	-55.5484587	-36.48480495	-19.06365376	-55.5484587
Ag tetrahedron + AA2 vertc - 11	-16.64235415	-55.28149421	-38.1834419	-17.09805232	-55.28149421
Ag tetrahedron + AA2 vertc - 12	-16.02314805	-54.66228811	-34.9549526	-19.70733551	-54.66228811
Ag tetrahedron + AA2 vertc - 13	-15.81161449	-54.45075454	-34.82408084	-19.6266737	-54.45075454
Ag tetrahedron + AA2 vertc - 14	-15.5656221	-54.20476216	-36.20511854	-17.99964362	-54.20476216
Ag tetrahedron + AA2 vertc - 15	-15.26055894	-53.899699	-35.26308102	-18.63661798	-53.899699
Ag tetrahedron + AA2 vertc - 16	-14.83952673	-53.47866679	-34.76914749	-18.7095193	-53.47866679
Ag tetrahedron + AA2 vertc - 17	-14.48358969	-53.12272974	-34.32784926	-18.79488048	-53.12272974
Ag tetrahedron + AA2 vertc - 18	-14.16141325	-52.80055331	-32.69023158	-20.11032173	-52.80055331
Ag tetrahedron + AA2 vertc - 19	-13.78578262	-52.42492267	-34.2421998	-18.18272287	-52.42492267
Ag tetrahedron + AA2 vertc - 20	-13.51767235	-52.1568124	-33.24926736	-18.90754504	-52.1568124
Ag tetrahedron + AA2 vertc - 21	-13.31399594	-51.953136	-32.2265923	-19.7265437	-51.953136
Ag tetrahedron + AA2 vertc - 22	-12.7403644	-51.37950445	-32.05671976	-19.32278469	-51.37950445
Ag tetrahedron + AA2 vertc - 23	-12.52397764	-51.16311769	-32.05728944	-19.10582825	-51.16311769
Ag tetrahedron + AA2 vertc - 24	-12.27112385	-50.91026391	-33.47646847	-17.43379544	-50.91026391
Ag tetrahedron + AA2 vertc - 25	-12.06477285	-50.7039129	-32.81713643	-17.88677648	-50.7039129
Ag tetrahedron + AA2 vertc - 26	-11.69914072	-50.33828078	-32.40764356	-17.93063722	-50.33828078

Ag tetrahedron + AA2 vertc - 27	-11.36671163	-50.00585169	-30.72223078	-19.28362091	-50.00585169
Ag tetrahedron + AA2 vertc - 28	-11.07243216	-49.71157221	-30.27253151	-19.43904071	-49.71157221
Ag tetrahedron + AA2 vertc - 29	-10.82174864	-49.4608887	-29.89191746	-19.56897124	-49.4608887
Ag tetrahedron + AA2 vertc - 30	-10.61952256	-49.25866262	-29.80136157	-19.45730105	-49.25866262
Ag tetrahedron + AA2 vertc - 31	-10.36022897	-48.99936903	-28.97376375	-20.02560528	-48.99936903
Ag tetrahedron + AA2 vertc - 32	-10.15926345	-48.79840351	-30.52359226	-18.27481125	-48.79840351
Ag tetrahedron + AA2 vertc - 33	-9.854776	-48.49391606	-30.20145644	-18.29245962	-48.49391606
Ag tetrahedron + AA2 vertc - 34	-9.48335427	-48.12249433	-28.66137936	-19.46111496	-48.12249433
Ag tetrahedron + AA2 vertc - 35	-8.93100274	-47.5701428	-28.59863055	-18.97151224	-47.5701428
Ag tetrahedron + AA2 vertc - 36	-8.50838956	-47.14752962	-28.73794535	-18.40958427	-47.14752962
Ag tetrahedron + AA2 vertc - 37	-8.29261387	-46.93175393	-28.82804955	-18.10370437	-46.93175393
Ag tetrahedron + AA2 vertc - 38	-7.86528879	-46.50442885	-28.86615215	-17.63827671	-46.50442885
Ag tetrahedron + AA2 vertc - 39	-7.37706802	-46.01620807	-25.95538062	-20.06082745	-46.01620807
Ag tetrahedron + AA2 vertc - 40	-6.86495676	-45.50409682	-27.46472923	-18.03936759	-45.50409682
Ag tetrahedron + AA2 vertc - 41	-6.52438592	-45.16352598	-26.61468318	-18.54884281	-45.16352598
Ag tetrahedron + AA2 vertc - 42	-6.19249903	-44.83163909	-24.74913139	-20.0825077	-44.83163909
Ag tetrahedron + AA2 vertc - 43	-5.61862517	-44.25776523	-25.69247888	-18.56528635	-44.25776523
Ag tetrahedron + AA2 vertc - 44	-4.56362508	-43.20276514	-23.89763213	-19.30513301	-43.20276514
Ag tetrahedron + AA2 vertc - 45	-4.24689642	-42.88603647	-22.76476143	-20.12127504	-42.88603647
Ag tetrahedron + AA2 vertc - 46	-3.87890078	-42.51804083	-22.96067051	-19.55737032	-42.51804083
Ag tetrahedron + AA2 vertc - 47	-3.64773966	-42.28687972	-22.76431418	-19.52256554	-42.28687972
Ag tetrahedron + AA2 vertc - 48	-3.44203671	-42.08117677	-22.62222712	-19.45894965	-42.08117677
Ag tetrahedron + AA2 vertc - 49	-2.65687459	-41.29601464	-21.74965688	-19.54635777	-41.29601464
Ag tetrahedron + AA2 vertc - 50	-1.21482163	-39.85396169	-19.59673705	-20.25722463	-39.85396169
Ag tetrahedron + AA2 vertc - 51	-0.679609	-39.31874906	-19.66052905	-19.65822001	-39.31874906
Ag tetrahedron + AA2 vertc - 52	-0.03536889	-38.67450895	-19.95974414	-18.71476481	-38.67450895
Ag tetrahedron + AA2 vertc - 53	1.35294013	-37.28619993	-17.02239021	-20.26380972	-37.28619993
Ag tetrahedron + AA2 vertc - 54	1.91179529	-36.72734476	-17.06169026	-19.66565451	-36.72734476
Ag tetrahedron + AA2 vertc - 55	2.82899245	-35.81014761	-16.29230394	-19.51784367	-35.81014761

Ag tetrahedron + AA2 vertc - 56	4.12962879	-34.50951127	-14.82522228	-19.68428899	-34.50951127

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Ascorbic acid(AA2)

Table A.17: Different configurations of Ag tetrahedron when the ascorbic acid (AA2) attached on the face.

Structures	TE	Ads	RAE	DE	AA2: dEad/dNi
Ag tetrahedron + AA2 face - 1	-17.31819558	-55.95733564	-36.91841542	-19.03892022	-55.95733564
Ag tetrahedron + AA2 face - 2	-16.61241747	-55.25155753	-35.03273359	-20.21882394	-55.25155753
Ag tetrahedron + AA2 face - 3	-16.09564866	-54.73478871	-35.1344032	-19.60038551	-54.73478871
Ag tetrahedron + AA2 face - 4	-15.33635337	-53.97549342	-35.62062167	-18.35487176	-53.97549342
Ag tetrahedron + AA2 face - 5	-14.98671202	-53.62585207	-35.74557148	-17.88028059	-53.62585207
Ag tetrahedron + AA2 face - 6	-14.73246588	-53.37160593	-35.94215457	-17.42945137	-53.37160593
Ag tetrahedron + AA2 face - 7	-14.22861613	-52.86775619	-32.70701756	-20.16073863	-52.86775619
Ag tetrahedron + AA2 face - 8	-13.64227253	-52.28141259	-32.76415053	-19.51726206	-52.28141259
Ag tetrahedron + AA2 face - 9	-13.33708431	-51.97622437	-33.03412594	-18.94209843	-51.97622437
Ag tetrahedron + AA2 face - 10	-13.13513485	-51.7742749	-32.58349946	-19.19077544	-51.7742749
Ag tetrahedron + AA2 face - 11	-12.73876035	-51.3779004	-31.79028169	-19.58761871	-51.3779004
Ag tetrahedron + AA2 face - 12	-12.50248227	-51.14162233	-31.29319831	-19.84842402	-51.14162233
Ag tetrahedron + AA2 face - 13	-12.0086931	-50.64783316	-31.68464063	-18.96319253	-50.64783316
Ag tetrahedron + AA2 face - 14	-11.79849554	-50.4376356	-31.38789378	-19.04974182	-50.4376356
Ag tetrahedron + AA2 face - 15	-11.57191862	-50.21105868	-31.32202337	-18.88903531	-50.21105868
Ag tetrahedron + AA2 face - 16	-11.35294762	-49.99208768	-30.68485155	-19.30723613	-49.99208768
Ag tetrahedron + AA2 face - 17	-11.05028506	-49.68942512	-30.03538557	-19.65403954	-49.68942512
Ag tetrahedron + AA2 face - 18	-10.84366499	-49.48280505	-34.0684912	-15.41431385	-49.48280505
Ag tetrahedron + AA2 face - 19	-10.61517216	-49.25431221	-29.43150837	-19.82280384	-49.25431221
Ag tetrahedron + AA2 face - 20	-10.40628846	-49.04542851	-30.19319805	-18.85223047	-49.04542851
Ag tetrahedron + AA2 face - 21	-9.86430524	-48.5034453	-28.39823031	-20.10521499	-48.5034453
Ag tetrahedron + AA2 face - 22	-9.61633393	-48.25547399	-29.06058887	-19.19488512	-48.25547399
Ag tetrahedron + AA2 face - 23	-9.22189835	-47.86103841	-28.35180322	-19.50923519	-47.86103841

Ag tetrahedron + AA2 face - 24	-8.76402713	-47.40316718	-31.69358169	-15.70958549	-47.40316718
Ag tetrahedron + AA2 face - 25	-8.5346027	-47.17374276	-28.0679057	-19.10583706	-47.17374276
Ag tetrahedron + AA2 face - 26	-8.20504695	-46.844187	-26.80299894	-20.04118807	-46.844187
Ag tetrahedron + AA2 face - 27	-7.27269254	-45.9118326	-27.46388569	-18.44794691	-45.9118326
Ag tetrahedron + AA2 face - 28	-7.02970981	-45.66884987	-27.38879792	-18.28005195	-45.66884987
Ag tetrahedron + AA2 face - 29	-6.75623792	-45.39537798	-27.10165738	-18.2937206	-45.39537798
Ag tetrahedron + AA2 face - 30	-5.83359796	-44.47273802	-26.39312549	-18.07961252	-44.47273802
Ag tetrahedron + AA2 face - 31	-4.41380061	-43.05294067	-24.3262431	-18.72669757	-43.05294067

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Ascorbic acid (AA2)

Table A.18: Different configurations of Ag tetrahedron when the ascorbic acid (AA2) attached on the edge.

Structures	TE	Ads	RAE	DE	AA2: dEad/dNi
Ag tetrahedron + AA2 edge - 1	-23.59230705	-62.23144711	-42.68360522	-19.54784189	-62.23144711
Ag tetrahedron + AA2 edge - 2	-22.82683949	-61.46597954	-42.45248253	-19.01349701	-61.46597954
Ag tetrahedron + AA2 edge - 3	-22.40694548	-61.04608554	-42.75673018	-18.28935536	-61.04608554
Ag tetrahedron + AA2 edge - 4	-21.96209307	-60.60123313	-43.14952672	-17.45170641	-60.60123313
Ag tetrahedron + AA2 edge - 5	-19.29579313	-57.93493319	-40.12279335	-17.81213984	-57.93493319
Ag tetrahedron + AA2 edge - 6	-18.66366713	-57.30280719	-39.08968913	-18.21311806	-57.30280719
Ag tetrahedron + AA2 edge - 7	-18.42935161	-57.06849167	-39.0578937	-18.01059797	-57.06849167
Ag tetrahedron + AA2 edge - 8	-18.21767704	-56.8568171	-39.78001147	-17.07680562	-56.8568171
Ag tetrahedron + AA2 edge - 9	-17.77479721	-56.41393727	-38.60644997	-17.8074873	-56.41393727
Ag tetrahedron + AA2 edge - 10	-17.44689359	-56.08603365	-37.49985768	-18.58617597	-56.08603365
Ag tetrahedron + AA2 edge - 11	-17.04225135	-55.6813914	-38.36410772	-17.31728368	-55.6813914
Ag tetrahedron + AA2 edge - 12	-16.6423542	-55.28149426	-38.18332215	-17.09817211	-55.28149426
Ag tetrahedron + AA2 edge - 13	-16.17407908	-54.81321914	-35.15782938	-19.65538975	-54.81321914
Ag tetrahedron + AA2 edge - 14	-15.81161465	-54.4507547	-34.82449602	-19.62625868	-54.4507547
Ag tetrahedron + AA2 edge - 15	-15.59111174	-54.2302518	-36.06197525	-18.16827655	-54.2302518
Ag tetrahedron + AA2 edge - 16	-15.26055891	-53.89969897	-35.26316397	-18.636535	-53.89969897
Ag tetrahedron + AA2 edge - 17	-15.05429753	-53.69343759	-35.18864321	-18.50479438	-53.69343759

Ag tetrahedron + AA2 edge - 18	-14.69826266	-53.33740272	-35.34657292	-17.9908298	-53.33740272
Ag tetrahedron + AA2 edge - 19	-14.46586237	-53.10500243	-33.97607606	-19.12892638	-53.10500243
Ag tetrahedron + AA2 edge - 20	-13.51767239	-52.15681244	-33.24923505	-18.90757739	-52.15681244
Ag tetrahedron + AA2 edge - 21	-13.31399589	-51.95313595	-32.2264689	-19.72666705	-51.95313595
Ag tetrahedron + AA2 edge - 22	-12.74036442	-51.37950448	-32.05671627	-19.3227882	-51.37950448
Ag tetrahedron + AA2 edge - 23	-12.52397741	-51.16311747	-32.05714812	-19.10596935	-51.16311747
Ag tetrahedron + AA2 edge - 24	-12.27112378	-50.91026384	-33.4762185	-17.43404533	-50.91026384
Ag tetrahedron + AA2 edge - 25	-11.82786383	-50.46700388	-32.84367768	-17.62332621	-50.46700388
Ag tetrahedron + AA2 edge - 26	-11.61797046	-50.25711051	-31.01733663	-19.23977389	-50.25711051
Ag tetrahedron + AA2 edge - 27	-11.26626503	-49.90540509	-30.28830176	-19.61710333	-49.90540509
Ag tetrahedron + AA2 edge - 28	-10.82174863	-49.46088869	-29.89193906	-19.56894963	-49.46088869
Ag tetrahedron + AA2 edge - 29	-10.50201919	-49.14115925	-30.72440822	-18.41675103	-49.14115925
Ag tetrahedron + AA2 edge - 30	-10.30120245	-48.9403425	-31.01394188	-17.92640063	-48.9403425
Ag tetrahedron + AA2 edge - 31	-10.0732786	-48.71241865	-31.07067394	-17.64174472	-48.71241865
Ag tetrahedron + AA2 edge - 32	-9.85477556	-48.49391562	-30.20121966	-18.29269596	-48.49391562
Ag tetrahedron + AA2 edge - 33	-9.29417877	-47.93331883	-30.07120311	-17.86211571	-47.93331883
Ag tetrahedron + AA2 edge - 34	-8.92006539	-47.55920544	-28.55300119	-19.00620426	-47.55920544
Ag tetrahedron + AA2 edge - 35	-8.70675975	-47.34589981	-29.19830399	-18.14759582	-47.34589981
Ag tetrahedron + AA2 edge - 36	-8.3714106	-47.01055066	-27.63485027	-19.37570039	-47.01055066
Ag tetrahedron + AA2 edge - 37	-7.68597262	-46.32511268	-28.33062668	-17.994486	-46.32511268
Ag tetrahedron + AA2 edge - 38	-7.30567938	-45.94481944	-27.85894182	-18.08587762	-45.94481944
Ag tetrahedron + AA2 edge - 39	-6.8649568	-45.50409686	-27.46471329	-18.03938357	-45.50409686
Ag tetrahedron + AA2 edge - 40	-6.26979465	-44.90893471	-25.97296163	-18.93597308	-44.90893471
Ag tetrahedron + AA2 edge - 41	-5.57912565	-44.21826571	-26.19676501	-18.0215007	-44.21826571
Ag tetrahedron + AA2 edge - 42	-5.14787886	-43.78701892	-30.03079169	-13.75622722	-43.78701892
Ag tetrahedron + AA2 edge - 43	-4.71617764	-43.3553177	-25.13929824	-18.21601946	-43.3553177
Ag tetrahedron + AA2 edge - 44	-4.24689639	-42.88603645	-22.76476638	-20.12127007	-42.88603645
Ag tetrahedron + AA2 edge - 45	-3.64350608	-42.28264614	-22.74806814	-19.534578	-42.28264614
Ag tetrahedron + AA2 edge - 46	-3.32322792	-41.96236798	-21.80972988	-20.1526381	-41.96236798

Ag tetrahedron + AA2 edge - 47	-2.65687448	-41.29601454	-21.74970213	-19.54631241	-41.29601454
Ag tetrahedron + AA2 edge - 48	-1.99154881	-40.63068887	-20.3664026	-20.26428627	-40.63068887
Ag tetrahedron + AA2 edge - 49	-1.3800094	-40.01914946	-20.35335442	-19.66579504	-40.01914946
Ag tetrahedron + AA2 edge - 50	-0.67960912	-39.31874918	-19.6605901	-19.65815908	-39.31874918
Ag tetrahedron + AA2 edge - 51	-0.03536902	-38.67450908	-19.95980723	-18.71470186	-38.67450908
Ag tetrahedron + AA2 edge - 52	1.91179507	-36.72734499	-17.06180131	-19.66554368	-36.72734499
Ag tetrahedron + AA2 edge - 53	2.8289924	-35.81014766	-16.29237618	-19.51777148	-35.81014766
Ag tetrahedron + AA2 edge - 54	4.24376958	-34.39537048	-15.30137435	-19.09399613	-34.39537048

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Ascorbic acid (AA2)

Table A.19: Different configurations of Ag sphere when the formic acid (FA1) attached.

Structures	**TE**	**Ads**	**RAE**	**DE**	**FA1: dEad/dNi**
Ag Sphere + FA - 1	-33.654709	-12.80646653	-12.09819216	-0.70827436	-12.80646653
Ag Sphere + FA - 2	-33.4268513	-12.57860885	-11.86969933	-0.70890952	-12.57860885
Ag Sphere + FA - 3	-33.1618932	-12.31365076	-11.60883316	-0.7048176	-12.31365076
Ag Sphere + FA - 4	-32.7602412	-11.91199873	-11.20546106	-0.70653767	-11.91199873
Ag Sphere + FA - 5	-31.2475501	-10.39930766	-9.6910212	-0.70828646	-10.39930766

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Formic acid(FA1)

Table A.20: Different configurations of Ag sphere when the acetic acid (AA1) attached.

Structures	**TE**	**Ads**	**RAE**	**DE**	**AA1 : dEad/dNi**
Ag Sphere +AA1 – 1	-61.3867774	-16.56451982	-15.51524594	-1.04927388	-16.56451982
Ag Sphere +AA1 – 2	-61.0521402	-16.22988268	-15.04350952	-1.18637316	-16.22988268
Ag Sphere +AA1 – 3	-60.7070878	-15.88483026	-14.68727102	-1.19755924	-15.88483026
Ag Sphere +AA1 – 4	-60.380041	-15.5577834	-14.33533187	-1.22245154	-15.5577834
Ag Sphere +AA1 – 5	-60.0128204	-15.19056282	-14.06040225	-1.13016057	-15.19056282
Ag Sphere +AA1 – 6	-59.5394232	-14.7171656	-13.61476084	-1.10240477	-14.7171656
Ag Sphere +AA1 – 7	-58.5932936	-13.77103602	-12.59124593	-1.17979008	-13.77103602

Ag Sphere +AA1 – 8	-58.0643773	-13.24211971	-12.31804084	-0.92407887	-13.24211971
Ag Sphere +AA1 – 9	-56.7686316	-11.94637403	-10.72046366	-1.22591038	-11.94637403
Ag Sphere +AA1 – 10	-55.8738479	-11.05159034	-9.83612694	-1.2154634	-11.05159034

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Acetic acid(AA1)

Table A.21: Different configurations of Ag sphere when the ascorbic acid (AA2) attached.

Structures	**TE**	**Ads**	**RAE**	**DE**	**AA2: dEad/dNi**
Ag Sphere +AA2 – 1	-9.78912849	-48.42826855	-28.72472122	-19.70354733	-48.42826855
Ag Sphere +AA2 – 2	-8.93348739	-47.57262744	-27.74933692	-19.82329052	-47.57262744
Ag Sphere +AA2 – 3	-8.56076106	-47.19990111	-27.85011109	-19.34979003	-47.19990111
Ag Sphere +AA2 – 4	-8.34908559	-46.98822565	-26.86550688	-20.12271877	-46.98822565
Ag Sphere +AA2 – 5	-7.91727915	-46.55641921	-27.92436089	-18.63205832	-46.55641921
Ag Sphere +AA2 – 6	-7.62541457	-46.26455463	-26.68769956	-19.57685507	-46.26455463
Ag Sphere +AA2 – 7	-7.21982382	-45.85896388	-26.81240618	-19.0465577	-45.85896388
Ag Sphere +AA2 – 8	-7.00151507	-45.64065513	-26.25909524	-19.38155989	-45.64065513
Ag Sphere +AA2 – 9	-6.59122266	-45.23036272	-25.61419329	-19.61616943	-45.23036272
Ag Sphere +AA2 – 10	-6.34602986	-44.98516992	-25.16142515	-19.82374477	-44.98516992
Ag Sphere +AA2 - 11	-5.86907773	-44.50821779	-26.62832071	-17.87989707	-44.50821779
Ag Sphere +AA2 - 12	-5.53225467	-44.17139473	-24.52699402	-19.6444007	-44.17139473
Ag Sphere +AA2 - 13	-5.15961206	-43.79875212	-25.00645681	-18.79229531	-43.79875212
Ag Sphere +AA2 - 14	-4.90343286	-43.54257292	-24.74423108	-18.79834183	-43.54257292
Ag Sphere +AA2 - 15	-4.62411327	-43.26325333	-23.68150301	-19.58175032	-43.26325333
Ag Sphere +AA2 - 16	-4.38684256	-43.02598262	-23.44131878	-19.58466385	-43.02598262
Ag Sphere +AA2 - 17	-4.10218248	-42.74132254	-24.61472202	-18.12660052	-42.74132254
Ag Sphere +AA2 - 18	-3.59455499	-42.23369505	-23.57208172	-18.66161333	-42.23369505
Ag Sphere +AA2 - 19	-2.98880463	-41.62794469	-21.43175415	-20.19619054	-41.62794469
Ag Sphere +AA2 - 20	-2.61805264	-41.2571927	-21.75136331	-19.50582938	-41.2571927

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Ascorbic acid (AA2)

Table A.22: Different configurations of Ag cylinder when the formic acid (FA1) attached.

Structures	TE	Ads	RAE	DE	FA1 : dEad/dNi
Ag cylinder + FA - 1	-36.44078966	-15.5925472	-14.88725846	-0.70528874	-15.5925472
Ag cylinder + FA - 2	-36.12533889	-15.27709642	-14.57307921	-0.70401721	-15.27709642
Ag cylinder + FA - 3	-32.14020322	-11.29196076	-10.58653877	-0.70542198	-11.29196076
Ag cylinder + FA - 4	-31.72318949	-10.87494703	-10.16685876	-0.70808827	-10.87494703
Ag cylinder + FA - 5	-30.50423564	-9.65599317	-8.94860223	-0.70739094	-9.65599317

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Formic acid(FA1)

Table A.23: Different configurations of Ag cylinder when the acetic acid (AA2) attached.

Structures	TE	Ads	RAE	DE	AA1: dEad/dNi
Ag cylinder + AA1 – 1	-65.10498365	-20.2827261	-19.18235151	-1.1003746	-20.2827261
Ag cylinder + AA1 – 2	-60.10773922	-15.28548167	-14.16729667	-1.118185	-15.28548167
Ag cylinder + AA1 – 3	-59.90337279	-15.08111524	-13.95291905	-1.12819619	-15.08111524
Ag cylinder + AA1 – 4	-59.27149463	-14.44923708	-13.24392711	-1.20530997	-14.44923708
Ag cylinder + AA1 – 5	-59.01863577	-14.19637822	-12.9923524	-1.20402582	-14.19637822
Ag cylinder + AA1 – 6	-57.4183807	-12.59612315	-11.38142766	-1.21469549	-12.59612315
Ag cylinder + AA1 – 7	-55.8696995	-11.04744195	-9.82369383	-1.22374812	-11.04744195

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Acetic acid(AA1)

Table A.24: Different configurations of Ag cylinder when the ascorbic acid (AA2) attached.

Structures	TE	Ads	RAE	DE	AA2: dEad/dNi
Ag cylinder + AA2 - 1	-8.61756874	-47.2567088	-28.4260847	-18.83062409	-47.2567088
Ag cylinder + AA2 - 2	-6.26302739	-44.90216745	-24.75342383	-20.14874362	-44.90216745
Ag cylinder + AA2 - 3	-5.74143871	-44.38057877	-24.21557442	-20.16500435	-44.38057877
Ag cylinder + AA2 - 4	-5.49574296	-44.13488302	-24.59377926	-19.54110376	-44.13488302
Ag cylinder + AA2 - 5	-5.09151534	-43.7306554	-24.18936776	-19.54128764	-43.7306554
Ag cylinder + AA2 - 6	-4.72126621	-43.36040627	-23.4035416	-19.95686466	-43.36040627
Ag cylinder + AA2 - 7	-4.51166345	-43.15080351	-23.19653989	-19.95426362	-43.15080351
Ag cylinder + AA2 - 8	-4.25602517	-42.89516523	-23.74910643	-19.1460588	-42.89516523
Ag cylinder + AA2 - 9	-4.03704244	-42.67618249	-23.14827068	-19.52791181	-42.67618249
Ag cylinder + AA2 - 10	-3.74773201	-42.38687207	-23.91217853	-18.47469354	-42.38687207
Ag cylinder + AA2 - 11	-3.54263702	-42.18177707	-23.57760081	-18.60417626	-42.18177707
Ag cylinder + AA2 - 12	-3.28008494	-41.919225	-23.27580289	-18.64342211	-41.919225
Ag cylinder + AA2 - 13	-2.96223164	-41.6013717	-23.71775022	-17.88362148	-41.6013717
Ag cylinder + AA2 - 14	-2.76124879	-41.40038885	-23.41767536	-17.98271349	-41.40038885
Ag cylinder + AA2 - 15	-1.59559768	-40.23473774	-21.04607521	-19.18866253	-40.23473774
Ag cylinder + AA2 - 16	-1.38763024	-40.0267703	-20.8631019	-19.1636684	-40.0267703
Ag cylinder + AA2 - 17	-1.13354337	-39.77268343	-21.14692962	-18.6257538	-39.77268343
Ag cylinder + AA2 - 18	-0.92952107	-39.56866113	-20.96483681	-18.60382432	-39.56866113
Ag cylinder + AA2 - 19	-0.63339611	-39.27253617	-20.62705318	-18.64548299	-39.27253617
Ag cylinder + AA2 - 20	-0.37169943	-39.01083948	-20.38427315	-18.62656634	-39.01083948
Ag cylinder + AA2 - 21	-0.14911632	-38.78825637	-19.22550973	-19.56274664	-38.78825637
Ag cylinder + AA2 - 22	0.23466363	-38.40447643	-18.22309377	-20.18138265	-38.40447643
Ag cylinder + AA2 - 23	0.55268418	-38.08645587	-17.81962893	-20.26682694	-38.08645587
Ag cylinder + AA2 - 24	0.77046593	-37.86867413	-18.17356204	-19.69511209	-37.86867413
Ag cylinder + AA2 - 25	1.19590791	-37.44323215	-17.7822316	-19.66100055	-37.44323215
Ag cylinder + AA2 - 26	2.00057109	-36.63856897	-16.56420591	-20.07436306	-36.63856897

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Ascorbic acid(AA2)

Table A.25: Different configurations of Ag (111) surface when the Cryptochrome (Cry) attached.

Structures	TE	Ads	RAE	DE	Cry: dEad/dNi
Ag (1 1 1)-Cry - 1	-115.624875	-110.1482173	-114.8215011	4.67328383	-110.1482173
Ag (1 1 1)-Cry - 2	-114.756276	-109.2796179	-114.1448183	4.86520046	-109.2796179
Ag (1 1 1)-Cry - 3	-114.110165	-108.6335071	-115.267312	6.63380494	-108.6335071
Ag (1 1 1)-Cry - 4	-113.836288	-108.3596299	-115.4070766	7.04744665	-108.3596299
Ag (1 1 1)-Cry - 5	-113.601121	-108.1244627	-115.3454881	7.22102538	-108.1244627
Ag (1 1 1)-Cry - 6	-113.006429	-107.5297708	-115.2086444	7.67887359	-107.5297708
Ag (1 1 1)-Cry - 7	-110.923475	-105.446817	-113.0689053	7.6220883	-105.446817
Ag (1 1 1)-Cry - 8	-110.68883	-105.2121719	-114.4361371	9.22396518	-105.2121719
Ag (1 1 1)-Cry - 9	-109.668217	-104.1915591	-112.7739221	8.58236294	-104.1915591
Ag (1 1 1)-Cry - 10	-109.393404	-103.9167457	-115.0473671	11.13062141	-103.9167457
Ag (1 1 1)-Cry - 11	-106.876683	-101.4000255	-110.7876519	9.38762638	-101.4000255
Ag (1 1 1)-Cry - 12	-106.043454	-100.5667957	-110.1987715	9.63197579	-100.5667957
Ag (1 1 1)-Cry - 13	-104.383477	-98.90681938	-111.4096741	12.50285477	-98.90681938
Ag (1 1 1)-Cry - 14	-101.609471	-96.13281293	-111.8971238	15.76431091	-96.13281293
Ag (1 1 1)-Cry - 15	-100.837504	-95.36084613	-108.3901161	13.02926995	-95.36084613
Ag (1 1 1)-Cry - 16	-100.615663	-95.13900516	-111.1677542	16.02874901	-95.13900516
Ag (1 1 1)-Cry - 17	-98.5900041	-93.11334611	-111.3366298	18.22328366	-93.11334611
Ag (1 1 1)-Cry - 18	-98.0400271	-92.5633691	-111.4008585	18.83748938	-92.5633691
Ag (1 1 1)-Cry - 19	-97.5950709	-92.11841294	-113.8085276	21.69011467	-92.11841294
Ag (1 1 1)-Cry - 20	-96.9889048	-91.51224685	-112.4337377	20.92149089	-91.51224685
Ag (1 1 1)-Cry - 21	-96.3471822	-90.87052419	-112.9877603	22.11723607	-90.87052419
Ag (1 1 1)-Cry - 22	-95.9077178	-90.43105981	-108.5584334	18.12737362	-90.43105981
Ag (1 1 1)-Cry - 23	-95.37982	-89.90316202	-114.4704251	24.56726305	-89.90316202
Ag (1 1 1)-Cry - 24	-95.0498702	-89.5732122	-108.9231026	19.34989036	-89.5732122
Ag (1 1 1)-Cry - 25	-93.931243	-88.45458506	-110.9297138	22.47512876	-88.45458506
Ag (1 1 1)-Cry - 26	-92.5029314	-87.02627348	-114.1823902	27.15611672	-87.02627348
Ag (1 1 1)-Cry - 27	-91.9931168	-86.51645887	-113.1513329	26.63487402	-86.51645887
Ag (1 1 1)-Cry - 28	-91.5004298	-86.02377179	-113.0594597	27.03568786	-86.02377179
Ag (1 1 1)-Cry - 29	-90.2196724	-84.74301442	-109.3668187	24.62380426	-84.74301442
Ag (1 1 1)-Cry - 30	-89.2342306	-83.75757268	-114.0678864	30.31031368	-83.75757268

Ag (1 1 1)-Cry - 31	-89.0092053	-83.53254735	-109.0679199	25.53537257	-83.53254735
Ag (1 1 1)-Cry - 32	-88.2987369	-82.82207897	-113.3596787	30.53759974	-82.82207897
Ag (1 1 1)-Cry - 33	-86.961911	-81.48525304	-107.0639553	25.57870224	-81.48525304
Ag (1 1 1)-Cry - 34	-86.716801	-81.24014304	-111.4666556	30.22651261	-81.24014304
Ag (1 1 1)-Cry - 35	-86.3218491	-80.84519115	-105.5638932	24.71870201	-80.84519115
Ag (1 1 1)-Cry - 36	-86.0908876	-80.61422962	-110.7954497	30.18122007	-80.61422962
Ag (1 1 1)-Cry - 37	-85.40178	-79.92512202	-110.917031	30.99190892	-79.92512202
Ag (1 1 1)-Cry - 38	-85.1640936	-79.68743559	-110.9251502	31.23771459	-79.68743559
Ag (1 1 1)-Cry - 39	-84.8673881	-79.39073014	-112.1120475	32.72131738	-79.39073014
Ag (1 1 1)-Cry - 40	-84.6664895	-79.18983152	-110.2694285	31.07959701	-79.18983152
Ag (1 1 1)-Cry - 41	-84.1695155	-78.69285753	-108.4855818	29.79272427	-78.69285753
Ag (1 1 1)-Cry - 42	-83.7334199	-78.2567619	-110.225092	31.9683301	-78.2567619
Ag (1 1 1)-Cry - 43	-83.0811741	-77.60451615	-109.70632	32.10180386	-77.60451615
Ag (1 1 1)-Cry - 44	-82.7914288	-77.31477085	-110.1030281	32.78825727	-77.31477085
Ag (1 1 1)-Cry - 45	-82.5562066	-77.07954864	-105.5401888	28.46064018	-77.07954864
Ag (1 1 1)-Cry - 46	-82.2601546	-76.78349667	-104.2737693	27.49027261	-76.78349667
Ag (1 1 1)-Cry - 47	-82.0345927	-76.55793474	-111.19632	34.63838528	-76.55793474
Ag (1 1 1)-Cry - 48	-81.6586057	-76.1819477	-110.0362144	33.85426665	-76.1819477
Ag (1 1 1)-Cry - 49	-81.1961129	-75.71945493	-111.273448	35.55399308	-75.71945493
Ag (1 1 1)-Cry - 50	-80.9724474	-75.49578945	-110.8008003	35.30501089	-75.49578945
Ag (1 1 1)-Cry - 51	-80.7247743	-75.24811635	-110.3417146	35.09359827	-75.24811635
Ag (1 1 1)-Cry - 52	-80.4525847	-74.9759267	-109.6510356	34.67510893	-74.9759267
Ag (1 1 1)-Cry - 53	-79.6807544	-74.20409641	-109.9650561	35.76095968	-74.20409641
Ag (1 1 1)-Cry - 54	-79.369321	-73.89266304	-102.8024087	28.90974561	-73.89266304
Ag (1 1 1)-Cry - 55	-79.0504624	-73.57380447	-99.78606807	26.2122636	-73.57380447
Ag (1 1 1)-Cry - 56	-78.59154	-73.11488204	-100.3957289	27.28084685	-73.11488204
Ag (1 1 1)-Cry - 57	-77.973638	-72.49698008	-102.4417839	29.94480383	-72.49698008
Ag (1 1 1)-Cry - 58	-77.6462265	-72.16956858	-97.82638679	25.65681821	-72.16956858
Ag (1 1 1)-Cry - 59	-77.3883019	-71.91164397	-97.7774324	25.86578843	-71.91164397
Ag (1 1 1)-Cry - 60	-77.1629453	-71.68628734	-97.41332803	25.72704069	-71.68628734
Ag (1 1 1)-Cry - 61	-76.836083	-71.35942504	-99.01921575	27.65979071	-71.35942504
Ag (1 1 1)-Cry - 62	-76.6331293	-71.15647132	-101.8364914	30.68002005	-71.15647132
Ag (1 1 1)-Cry - 63	-76.1289062	-70.65224823	-97.3541694	26.70192117	-70.65224823
Ag (1 1 1)-Cry - 64	-75.7319658	-70.25530787	-105.622983	35.36767517	-70.25530787
Ag (1 1 1)-Cry - 65	-75.3977981	-69.92114015	-100.3725695	30.4514293	-69.92114015
Ag (1 1 1)-Cry - 66	-75.0708851	-69.59422709	-95.41192906	25.81770196	-69.59422709
Ag (1 1 1)-Cry - 67	-74.4492234	-68.97256545	-107.8510222	38.87845679	-68.97256545

Ag (1 1 1)-Cry - 68	-74.2339183	-68.75726029	-107.3831017	38.62584138	-68.75726029
Ag (1 1 1)-Cry - 69	-74.0165844	-68.53992648	-99.13311231	30.59318583	-68.53992648
Ag (1 1 1)-Cry - 70	-73.5999128	-68.12325486	-106.7461267	38.62287187	-68.12325486
Ag (1 1 1)-Cry - 71	-73.3653527	-67.88869471	-97.66618837	29.77749365	-67.88869471
Ag (1 1 1)-Cry - 72	-73.0533903	-67.57673233	-92.84924952	25.27251719	-67.57673233
Ag (1 1 1)-Cry - 73	-72.8360642	-67.35940626	-97.53895892	30.17955266	-67.35940626
Ag (1 1 1)-Cry - 74	-72.537171	-67.06051303	-92.9798165	25.91930347	-67.06051303
Ag (1 1 1)-Cry - 75	-72.1725494	-66.69589148	-104.7768571	38.08096556	-66.69589148
Ag (1 1 1)-Cry - 76	-71.9678132	-66.49115524	-90.98642812	24.49527288	-66.49115524
Ag (1 1 1)-Cry - 77	-71.7027444	-66.22608641	-91.20433811	24.97825171	-66.22608641
Ag (1 1 1)-Cry - 78	-71.2489539	-65.77229598	-94.09307524	28.32077926	-65.77229598
Ag (1 1 1)-Cry - 79	-70.9700634	-65.49340546	-91.20841208	25.71500662	-65.49340546
Ag (1 1 1)-Cry - 80	-70.7632643	-65.28660633	-90.72347936	25.43687303	-65.28660633
Ag (1 1 1)-Cry - 81	-70.3596569	-64.88299894	-92.32603284	27.44303391	-64.88299894
Ag (1 1 1)-Cry - 82	-69.6021703	-64.12551234	-99.127238	35.00172567	-64.12551234
Ag (1 1 1)-Cry - 83	-67.9215309	-62.44487297	-95.19706884	32.75219588	-62.44487297
Ag (1 1 1)-Cry - 84	-67.012841	-61.53618304	-91.91594455	30.37976151	-61.53618304
Ag (1 1 1)-Cry - 85	-66.410262	-60.93360403	-96.39358644	35.45998241	-60.93360403
Ag (1 1 1)-Cry - 86	-66.2071067	-60.73044878	-100.5124216	39.78197286	-60.73044878
Ag (1 1 1)-Cry - 87	-65.9997996	-60.52314168	-91.00316711	30.48002543	-60.52314168
Ag (1 1 1)-Cry - 88	-65.7742268	-60.29756887	-90.49390775	30.19633887	-60.29756887
Ag (1 1 1)-Cry - 89	-65.5256141	-60.04895611	-89.67266714	29.62371103	-60.04895611
Ag (1 1 1)-Cry - 90	-65.3121555	-59.83549751	-92.48358422	32.6480867	-59.83549751
Ag (1 1 1)-Cry - 91	-65.0199073	-59.54324935	-96.15723035	36.61398099	-59.54324935
Ag (1 1 1)-Cry - 92	-64.7411459	-59.26448797	-100.9199078	41.65541979	-59.26448797
Ag (1 1 1)-Cry - 93	-64.151504	-58.67484605	-91.46133021	32.78648417	-58.67484605
Ag (1 1 1)-Cry - 94	-61.1109642	-55.63430625	-93.38619424	37.751888	-55.63430625
Ag (1 1 1)-Cry - 95	-59.2325176	-53.75585966	-88.75568704	34.99982738	-53.75585966
Ag (1 1 1)-Cry - 96	-56.879932	-51.40327399	-88.94631204	37.54303805	-51.40327399
Ag (1 1 1)-Cry - 97	-53.028833	-47.55217504	-88.49097567	40.93880064	-47.55217504
Ag (1 1 1)-Cry - 98	-48.958122	-43.48146405	-87.35873964	43.87727559	-43.48146405
Ag (1 1 1)-Cry - 99	-48.0383727	-42.56171474	-73.25978132	30.69806658	-42.56171474

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Cryptochrome (Cry)

Table A.26: The calculated (ΔN) number of electrons transferred using equation 5.1

	Sphere	Cylinder	Tetrahedron
Ascorbic acid	3.11	3.22	3.26
Acetic acid	3.75	3.89	3.93
Formic acid	3.69	3.83	3.87

Appendix B

Case study 2: Case study 2: Adsorption of natural organic matter on Ag (111) surface using DFT-D.

Table B. 1: Different configurations of Ag (111) surface when the humic acid (HA) attached.

Structures	TE	Ads	RAE	DE	HA : dEad/dNi
Ag (1 1 1) - HA – 1	-88.41347695	-56.3307041	-52.39083006	-3.93987404	-56.3307041
Ag (1 1 1) - HA – 2	-87.52285793	-55.44008508	-51.2763182	-4.16376689	-55.44008508
Ag (1 1 1) - HA – 3	-86.15482559	-54.07205274	-50.96427754	-3.1077752	-54.07205274
Ag (1 1 1) - HA – 4	-85.63139618	-53.54862333	-51.12447727	-2.42414606	-53.54862333
Ag (1 1 1) - HA – 5	-85.12517125	-53.0423984	-50.48748142	-2.55491698	-53.0423984
Ag (1 1 1) - HA – 6	-82.07101686	-49.98824401	-46.92638239	-3.06186162	-49.98824401
Ag (1 1 1) - HA – 7	-81.71607329	-49.63330044	-44.40145749	-5.23184295	-49.63330044
Ag (1 1 1) - HA – 8	-72.17580897	-40.09303612	-34.94043196	-5.15260416	-40.09303612
Ag (1 1 1) - HA – 9	-68.72289303	-36.64012018	-31.37288558	-5.2672346	-36.64012018
Ag (1 1 1) - HA – 10	-67.98793178	-35.90515893	-30.39162918	-5.51352974	-35.90515893

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Humic acid (HA

Table B.2: Different configurations of Ag (111) surface when the Fulvic acid (FA2) attached.

Structures	TE	Ads	RAE	DE	FA2: dEad/dNi
Ag (1 1 1) - FA2 – 1	-201.2359108	-76.78673292	-77.68869271	0.90195979	-76.78673292
Ag (1 1 1) - FA2- 2	-192.6300085	-68.18083066	-65.96185562	-2.21897504	-68.18083066
Ag (1 1 1) - FA2 – 3	-191.6469728	-67.19779496	-64.70737511	-2.49041985	-67.19779496
Ag (1 1 1) - FA2 – 4	-191.3022834	-66.85310557	-64.42623441	-2.42687115	-66.85310557
Ag (1 1 1) - FA2 – 5	-187.0468953	-62.59771747	-55.32521056	-7.27250691	-62.59771747
Ag (1 1 1) - FA2 – 6	-185.9177708	-61.4685929	-54.1361556	-7.3324373	-61.4685929
Ag (1 1 1) - FA2 – 7	-176.9787095	-52.52953165	-58.49132625	5.96179459	-52.52953165

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Fulvic acid (FA2)

Table B.3: Different configurations of Ag (111) surface when the cryptochrome (Cry) attached.

Structures	TE	Ads	RAE	DE	Cry: dEad/dNi
Ag (1 1 1)-Cry - 1	-115.624875	-110.1482173	-114.8215011	4.67328383	-110.1482173
Ag (1 1 1)-Cry - 2	-114.756276	-109.2796179	-114.1448183	4.86520046	-109.2796179
Ag (1 1 1)-Cry - 3	-114.110165	-108.6335071	-115.267312	6.63380494	-108.6335071
Ag (1 1 1)-Cry - 4	-113.836288	-108.3596299	-115.4070766	7.04744665	-108.3596299
Ag (1 1 1)-Cry - 5	-113.601121	-108.1244627	-115.3454881	7.22102538	-108.1244627
Ag (1 1 1)-Cry - 6	-113.006429	-107.5297708	-115.2086444	7.67887359	-107.5297708
Ag (1 1 1)-Cry - 7	-110.923475	-105.446817	-113.0689053	7.6220883	-105.446817
Ag (1 1 1)-Cry - 8	-110.68883	-105.2121719	-114.4361371	9.22396518	-105.2121719
Ag (1 1 1)-Cry - 9	-109.668217	-104.1915591	-112.7739221	8.58236294	-104.1915591
Ag (1 1 1)-Cry - 10	-109.393404	-103.9167457	-115.0473671	11.13062141	-103.9167457
Ag (1 1 1)-Cry - 11	-106.876683	-101.4000255	-110.7876519	9.38762638	-101.4000255
Ag (1 1 1)-Cry - 12	-106.043454	-100.5667957	-110.1987715	9.63197579	-100.5667957
Ag (1 1 1)-Cry - 13	-104.383477	-98.90681938	-111.4096741	12.50285477	-98.90681938
Ag (1 1 1)-Cry - 14	-101.609471	-96.13281293	-111.8971238	15.76431091	-96.13281293
Ag (1 1 1)-Cry - 15	-100.837504	-95.36084613	-108.3901161	13.02926995	-95.36084613
Ag (1 1 1)-Cry - 16	-100.615663	-95.13900516	-111.1677542	16.02874901	-95.13900516
Ag (1 1 1)-Cry - 17	-98.5900041	-93.11334611	-111.3366298	18.22328366	-93.11334611
Ag (1 1 1)-Cry - 18	-98.0400271	-92.5633691	-111.4008585	18.83748938	-92.5633691
Ag (1 1 1)-Cry - 19	-97.5950709	-92.11841294	-113.8085276	21.69011467	-92.11841294
Ag (1 1 1)-Cry - 20	-96.9889048	-91.51224685	-112.4337377	20.92149089	-91.51224685
Ag (1 1 1)-Cry - 21	-96.3471822	-90.87052419	-112.9877603	22.11723607	-90.87052419
Ag (1 1 1)-Cry - 22	-95.9077178	-90.43105981	-108.5584334	18.12737362	-90.43105981
Ag (1 1 1)-Cry - 23	-95.37982	-89.90316202	-114.4704251	24.56726305	-89.90316202
Ag (1 1 1)-Cry - 24	-95.0498702	-89.5732122	-108.9231026	19.34989036	-89.5732122
Ag (1 1 1)-Cry - 25	-93.931243	-88.45458506	-110.9297138	22.47512876	-88.45458506

Ag (1 1 1)-Cry - 26	-92.5029314	-87.02627348	-114.1823902	27.15611672	-87.02627348
Ag (1 1 1)-Cry - 27	-91.9931168	-86.51645887	-113.1513329	26.63487402	-86.51645887
Ag (1 1 1)-Cry - 28	-91.5004298	-86.02377179	-113.0594597	27.03568786	-86.02377179
Ag (1 1 1)-Cry - 29	-90.2196724	-84.74301442	-109.3668187	24.62380426	-84.74301442
Ag (1 1 1)-Cry - 30	-89.2342306	-83.75757268	-114.0678864	30.31031368	-83.75757268
Ag (1 1 1)-Cry - 31	-89.0092053	-83.53254735	-109.0679199	25.53537257	-83.53254735
Ag (1 1 1)-Cry - 32	-88.2987369	-82.82207897	-113.3596787	30.53759974	-82.82207897
Ag (1 1 1)-Cry - 33	-86.961911	-81.48525304	-107.0639553	25.57870224	-81.48525304
Ag (1 1 1)-Cry - 34	-86.716801	-81.24014304	-111.4666556	30.22651261	-81.24014304
Ag (1 1 1)-Cry - 35	-86.3218491	-80.84519115	-105.5638932	24.71870201	-80.84519115
Ag (1 1 1)-Cry - 36	-86.0908876	-80.61422962	-110.7954497	30.18122007	-80.61422962
Ag (1 1 1)-Cry - 37	-85.40178	-79.92512202	-110.917031	30.99190892	-79.92512202
Ag (1 1 1)-Cry - 38	-85.1640936	-79.68743559	-110.9251502	31.23771459	-79.68743559
Ag (1 1 1)-Cry - 39	-84.8673881	-79.39073014	-112.1120475	32.72131738	-79.39073014
Ag (1 1 1)-Cry - 40	-84.6664895	-79.18983152	-110.2694285	31.07959701	-79.18983152
Ag (1 1 1)-Cry - 41	-84.1695155	-78.69285753	-108.4855818	29.79272427	-78.69285753
Ag (1 1 1)-Cry - 42	-83.7334199	-78.2567619	-110.225092	31.9683301	-78.2567619
Ag (1 1 1)-Cry - 43	-83.0811741	-77.60451615	-109.70632	32.10180386	-77.60451615
Ag (1 1 1)-Cry - 44	-82.7914288	-77.31477085	-110.1030281	32.78825727	-77.31477085
Ag (1 1 1)-Cry - 45	-82.5562066	-77.07954864	-105.5401888	28.46064018	-77.07954864
Ag (1 1 1)-Cry - 46	-82.2601546	-76.78349667	-104.2737693	27.49027261	-76.78349667
Ag (1 1 1)-Cry - 47	-82.0345927	-76.55793474	-111.19632	34.63838528	-76.55793474
Ag (1 1 1)-Cry - 48	-81.6586057	-76.1819477	-110.0362144	33.85426665	-76.1819477
Ag (1 1 1)-Cry - 49	-81.1961129	-75.71945493	-111.273448	35.55399308	-75.71945493
Ag (1 1 1)-Cry - 50	-80.9724474	-75.49578945	-110.8008003	35.30501089	-75.49578945
Ag (1 1 1)-Cry - 51	-80.7247743	-75.24811635	-110.3417146	35.09359827	-75.24811635
Ag (1 1 1)-Cry - 52	-80.4525847	-74.9759267	-109.6510356	34.67510893	-74.9759267
Ag (1 1 1)-Cry - 53	-79.6807544	-74.20409641	-109.9650561	35.76095968	-74.20409641
Ag (1 1 1)-Cry - 54	-79.369321	-73.89266304	-102.8024087	28.90974561	-73.89266304

Ag (1 1 1)-Cry - 55	-79.0504624	-73.57380447	-99.78606807	26.2122636	-73.57380447
Ag (1 1 1)-Cry - 56	-78.59154	-73.11488204	-100.3957289	27.28084685	-73.11488204
Ag (1 1 1)-Cry - 57	-77.973638	-72.49698008	-102.4417839	29.94480383	-72.49698008
Ag (1 1 1)-Cry - 58	-77.6462265	-72.16956858	-97.82638679	25.65681821	-72.16956858
Ag (1 1 1)-Cry - 59	-77.3883019	-71.91164397	-97.7774324	25.86578843	-71.91164397
Ag (1 1 1)-Cry - 60	-77.1629453	-71.68628734	-97.41332803	25.72704069	-71.68628734
Ag (1 1 1)-Cry - 61	-76.836083	-71.35942504	-99.01921575	27.65979071	-71.35942504
Ag (1 1 1)-Cry - 62	-76.6331293	-71.15647132	-101.8364914	30.68002005	-71.15647132
Ag (1 1 1)-Cry - 63	-76.1289062	-70.65224823	-97.3541694	26.70192117	-70.65224823
Ag (1 1 1)-Cry - 64	-75.7319658	-70.25530787	-105.622983	35.36767517	-70.25530787
Ag (1 1 1)-Cry - 65	-75.3977981	-69.92114015	-100.3725695	30.4514293	-69.92114015
Ag (1 1 1)-Cry - 66	-75.0708851	-69.59422709	-95.41192906	25.81770196	-69.59422709
Ag (1 1 1)-Cry - 67	-74.4492234	-68.97256545	-107.8510222	38.87845679	-68.97256545
Ag (1 1 1)-Cry - 68	-74.2339183	-68.75726029	-107.3831017	38.62584138	-68.75726029
Ag (1 1 1)-Cry - 69	-74.0165844	-68.53992648	-99.13311231	30.59318583	-68.53992648
Ag (1 1 1)-Cry - 70	-73.5999128	-68.12325486	-106.7461267	38.62287187	-68.12325486
Ag (1 1 1)-Cry - 71	-73.3653527	-67.88869471	-97.66618837	29.77749365	-67.88869471
Ag (1 1 1)-Cry - 72	-73.0533903	-67.57673233	-92.84924952	25.27251719	-67.57673233
Ag (1 1 1)-Cry - 73	-72.8360642	-67.35940626	-97.53895892	30.17955266	-67.35940626
Ag (1 1 1)-Cry - 74	-72.537171	-67.06051303	-92.9798165	25.91930347	-67.06051303
Ag (1 1 1)-Cry - 75	-72.1725494	-66.69589148	-104.7768571	38.08096556	-66.69589148
Ag (1 1 1)-Cry - 76	-71.9678132	-66.49115524	-90.98642812	24.49527288	-66.49115524
Ag (1 1 1)-Cry - 77	-71.7027444	-66.22608641	-91.20433811	24.97825171	-66.22608641
Ag (1 1 1)-Cry - 78	-71.2489539	-65.77229598	-94.09307524	28.32077926	-65.77229598
Ag (1 1 1)-Cry - 79	-70.9700634	-65.49340546	-91.20841208	25.71500662	-65.49340546
Ag (1 1 1)-Cry - 80	-70.7632643	-65.28660633	-90.72347936	25.43687303	-65.28660633
Ag (1 1 1)-Cry - 81	-70.3596569	-64.88299894	-92.32603284	27.44303391	-64.88299894
Ag (1 1 1)-Cry - 82	-69.6021703	-64.12551234	-99.127238	35.00172567	-64.12551234
Ag (1 1 1)-Cry - 83	-67.9215309	-62.44487297	-95.19706884	32.75219588	-62.44487297

Ag (1 1 1)-Cry - 84	-67.012841	-61.53618304	-91.91594455	30.37976151	-61.53618304
Ag (1 1 1)-Cry - 85	-66.410262	-60.93360403	-96.39358644	35.45998241	-60.93360403
Ag (1 1 1)-Cry - 86	-66.2071067	-60.73044878	-100.5124216	39.78197286	-60.73044878
Ag (1 1 1)-Cry - 87	-65.9997996	-60.52314168	-91.00316711	30.48002543	-60.52314168
Ag (1 1 1)-Cry - 88	-65.7742268	-60.29756887	-90.49390775	30.19633887	-60.29756887
Ag (1 1 1)-Cry - 89	-65.5256141	-60.04895611	-89.67266714	29.62371103	-60.04895611
Ag (1 1 1)-Cry - 90	-65.3121555	-59.83549751	-92.48358422	32.6480867	-59.83549751
Ag (1 1 1)-Cry - 91	-65.0199073	-59.54324935	-96.15723035	36.61398099	-59.54324935
Ag (1 1 1)-Cry - 92	-64.7411459	-59.26448797	-100.9199078	41.65541979	-59.26448797
Ag (1 1 1)-Cry - 93	-64.151504	-58.67484605	-91.46133021	32.78648417	-58.67484605
Ag (1 1 1)-Cry - 94	-61.1109642	-55.63430625	-93.38619424	37.751888	-55.63430625
Ag (1 1 1)-Cry - 95	-59.2325176	-53.75585966	-88.75568704	34.99982738	-53.75585966
Ag (1 1 1)-Cry - 96	-56.879932	-51.40327399	-88.94631204	37.54303805	-51.40327399
Ag (1 1 1)-Cry - 97	-53.028833	-47.55217504	-88.49097567	40.93880064	-47.55217504
Ag (1 1 1)-Cry - 98	-48.958122	-43.48146405	-87.35873964	43.87727559	-43.48146405
Ag (1 1 1)-Cry - 99	-48.0383727	-42.56171474	-73.25978132	30.69806658	-42.56171474

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Cryptochrome (Cry).

Structural properties

The interatomic bonds of the HA, FA, and Cry molecules were calculated and compared before and after relaxation as summarized in Table B.4. From the results, (Table B.4) insignificantly small differences were noted for bond distances before and after relaxation. To the authors' knowledge, no previous theoretical and experimental studies on reported bond lengths of HA, FA and Cry to allow one to make a comparison results derived from this study. It should be noted the bond lengths were unchanged in the gas phase and water as a solvent without and with dispersion corrections. Generally, as the adsorption energy increases with increasing MW, we expected the geometrical parameters in this case the distance between C-H, C-C, O-H and C-O to be influenced by the MW and the solvent effects. However, a comparison of Cry bond lengths to compared to HA and FA, no such influence was apparent.

Table B.4: Bond lengths of HA, FA and Cry before and after relaxation.

Adsorbate	**d_{C-H} (Å)**	**d_{C-C} (Å)**	**d_{O-H} (Å)**	**d_{C-O} (Å)**
Before relaxation				
HA	1.09	1.55	0.98	1.36
FA	1.08	1.39	0.97	1.36
Cry	1.08	1.45	0.97	1.43
After relaxation				
DFT-D gas phase				
HA	1.09	1.55	0.98	1.36
FA	1.08	1.39	0.97	1.36
Cry	1.08	1.45	0.97	1.42
DFT-D COSMO				
HA	1.09	1.55	0.98	1.36
FA	1.08	1.39	0.98	1.36
Cry	1.08	1.45	0.97	1.43

Abbreviation: d_{C-H}: is the distance between carbon and hydrogen, d_{C-C}: distance between carbon and carbon, d_{O-H}: is the distance between oxygen and hydrogen, and d_{C-O}: distance between carbon and oxygen.

Electronic properties

PDOS in Figures B.2-B.3 HA show intense peaks below and above Fermi level, prominent shoulder peaks corresponding to separate energy levels at -0.7 eV and -9.9 eV below the Fermi level and 4.3 eV and 4.8 eV above the Fermi level. PDOS in Figures B.2-B.3 FA shows prominent shoulder peaks at -4.1 eV and -9.9 eV, we also observed should mini peaks at around 2.9 eV and 4.8 eV above Fermi level. When the adsorbate and the adsorbent i.e Ag (111) surface in this case brought together, they start to interact. The adsorbate wave functions are hybridized and the s-band states of the substrate give rise to a broadening of the adsorbate levels. The electron chemical potential of the atom becomes aligned, as the atomic levels will shift to the substrate Fermi level. The broadening shifting of electronic levels is the first modification occurring as an atom is brought close to a surface, due to the spill out of the substrate s-electrons mostly into the vacuum (Scheffler and Stampfl 2000). The series of TDOS and PDOS plots, which apparently seem similar, illustrate some of the typical characteristics observed in the present study. Changes in the TDOS and PDOS features are a measure of the interaction between HA, FA and Cry on Ag (111) surface.

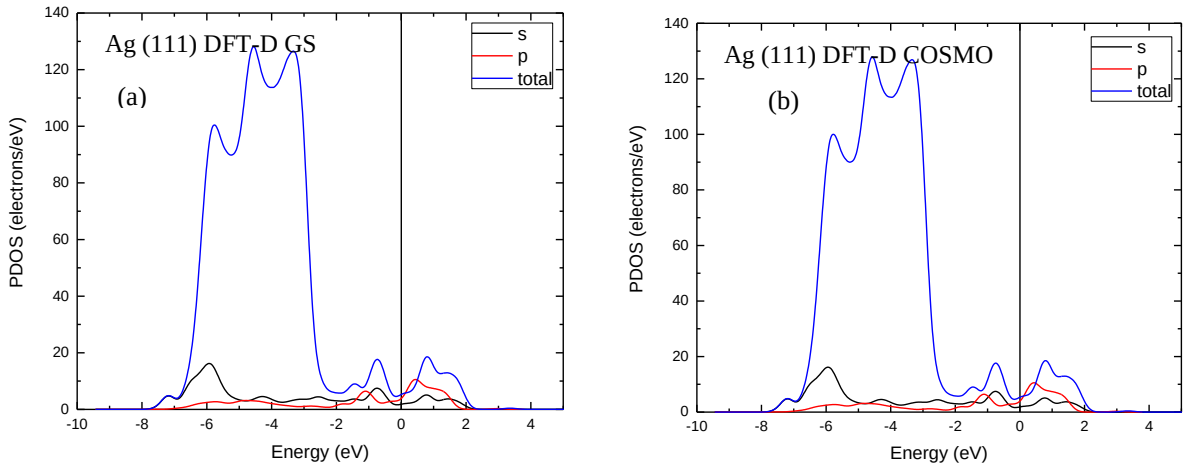


Figure B.1: Projected density of states of pristine of Ag (111) surface (a-b) in gas phase and COSMO using DFT-D/GGA.

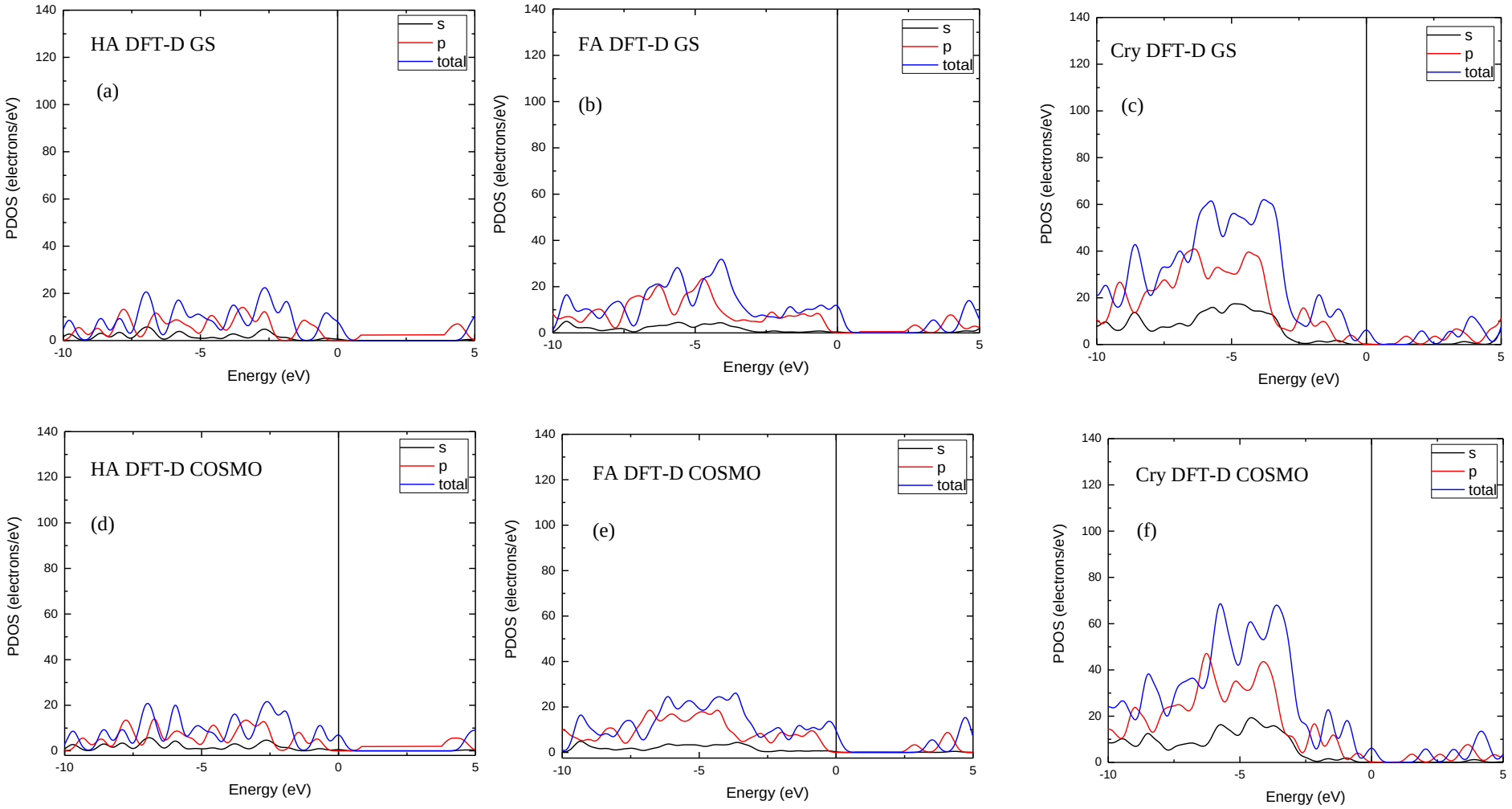


Figure B.2: Projected density of states of HA, FA and Cry (a-f) in gas phase and COSMO using DFT-D/GGA level of theory.

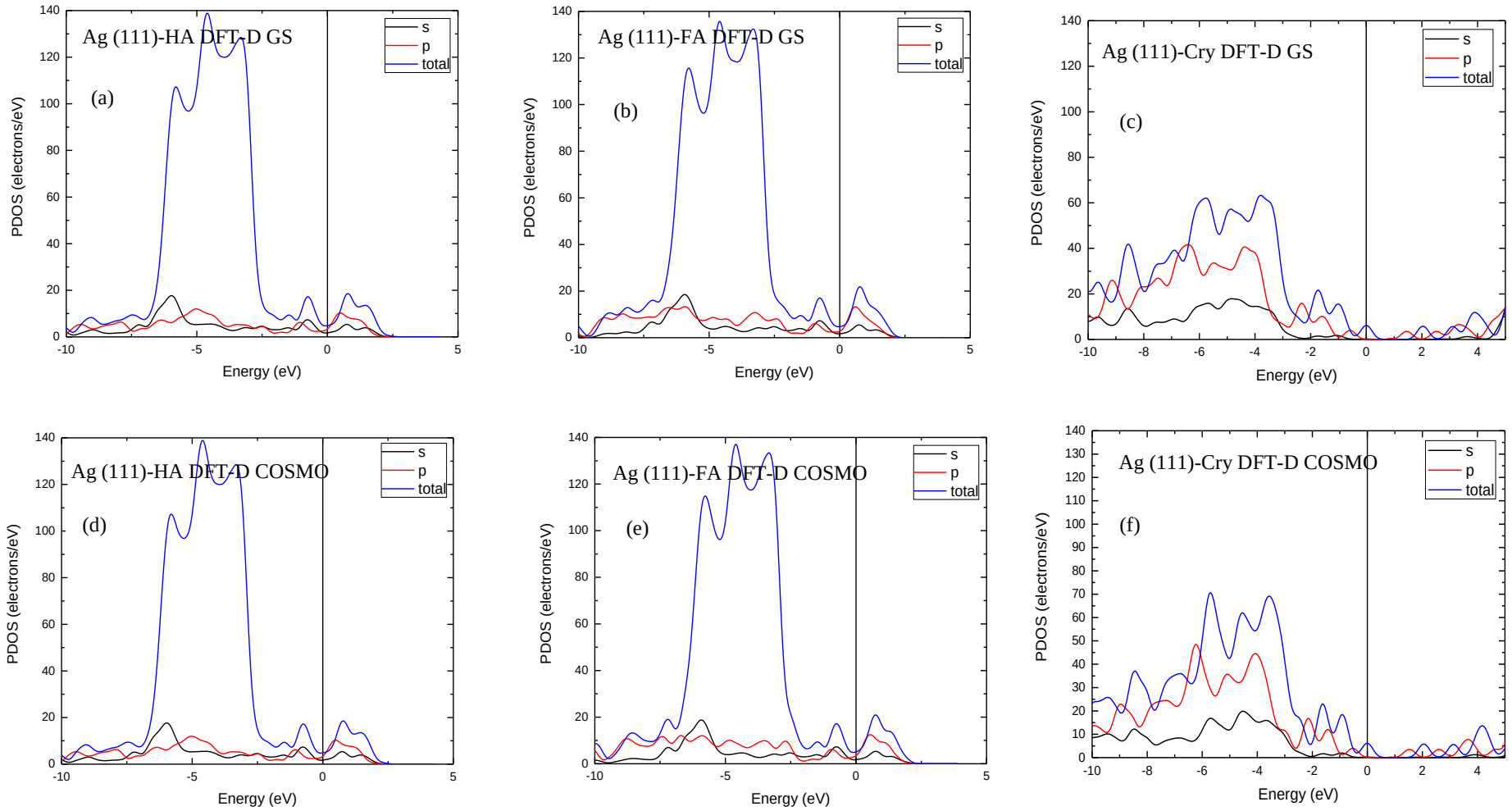


Figure B.3: Projected density of states of HA, FA and Cry on Ag (111) surface (a-f) in gas phase and COSMO using DFT-D/GGA level of theory.

Charge deformation difference of adsorbates

The adsorption of the three NOMs on Ag (111) surface lead to charge redistribution due to electronic hybridization between the adsorbates and the adsorbent orbitals (Chilukuri, Mazur, and Hipps 2014). To better understand the distribution patterns of charges around the adsorbates, results on charge density were plotted in three dimensional (3D) images based on charge density difference at the interfaces of HA, FA, and Cry on Ag (111) surface as shown in Figure B.4. For the FA and Cry shown in Figure B.4 (b) and (c), respectively, a strong redistribution of charges between C=O, C-C, C-H and -OH group was observed, and plausibly could yield a change in electron structure. The 3D iso-surfaces Figure B.4 (b-d) of charge redistribution at the interface indicate that the charge was localized mostly on the HA, FA, and Cry with smaller amounts on the pristine Ag (111) surface Figure B.4 (a).

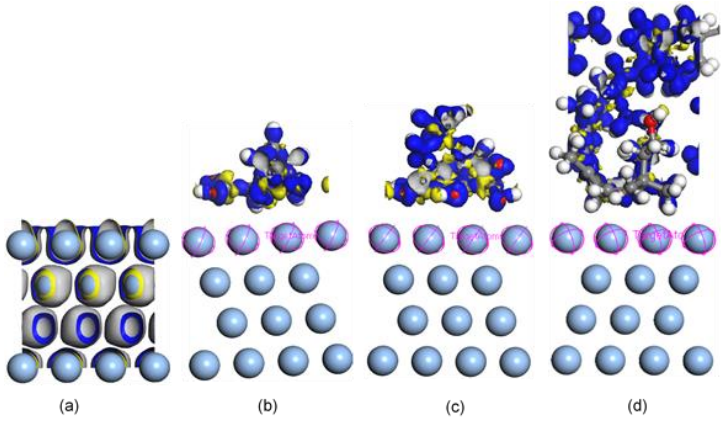


Figure B.4: Isosurface charge density difference for (a) Ag (111) pristine, (b) Ag (111)-HA, (c) Ag (111)-FA, and (d) Ag (111)-Cry derived using DFT-D COSMO level of theory. The isovalue is taken as for Ag (111) pristine 0.009 au to -0.009 au and 0.09 to -0.09 au for the rest. Blue region(s) indicates charge accumulation, and yellow region(s) show areas with charge depletion.

Another significant finding from the charge redistribution analysis is that dispersion interactions play a significant role in altering the charge redistribution on Ag (111) surface than on HA, FA and Cry. For the adsorption of NOM‘s on Ag (111) surface in Figure B.4 (b-d), the charge distribution on HA, FA and Cry is larger than that of the Ag (111) surface slab (see evidence shown by no color displacement on the slab after the adsorption. In addition, results in Figures B.5-B.7 (a) clearly show that regions with oxygen atom had higher charges, and hence the functional group likely to exert strong influence on the Ag (111) surface.

It should, however, be noted that this does not necessary suggest net charge transfer (Chilukuri, Mazur, and Hipps 2014) between adsorbates and Ag (111) surface, but rather

evidence of plausible charge transfer between surface and the adsorbates. The isosurface charge density difference for (a) Ag (111) pristine, (b) Ag (111)-HA, (c) Ag (111)-FA and (d) Ag (111)-Cry were the same irrespective of formalism used to perform the calculations (Figures B.8-B.11).

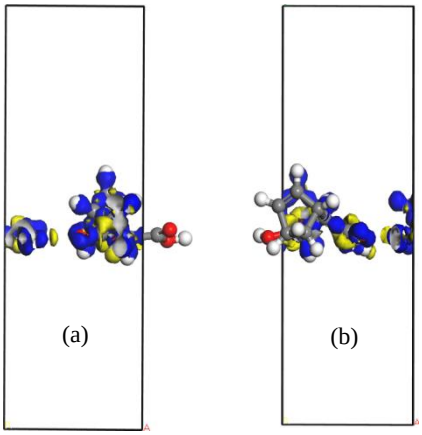


Figure B.5: Charge density difference for (a) HA at DFT-D COSMO level of theory, (b) HA at DFT-D gas phase level of theory. The isovalue is taken as 0.009 au.

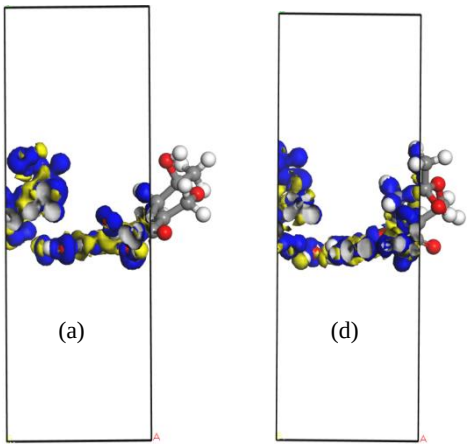


Figure B.6: Charge density difference for (a) FA at DFT-D COSMO level of theory, (b) FA at DFT-D gas phase level of theory. The isovalue is taken as 0.009 au.

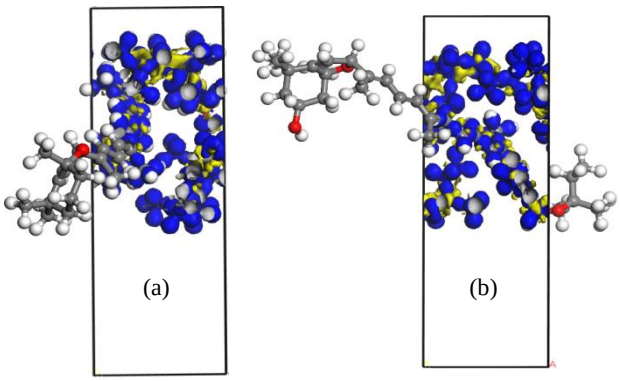
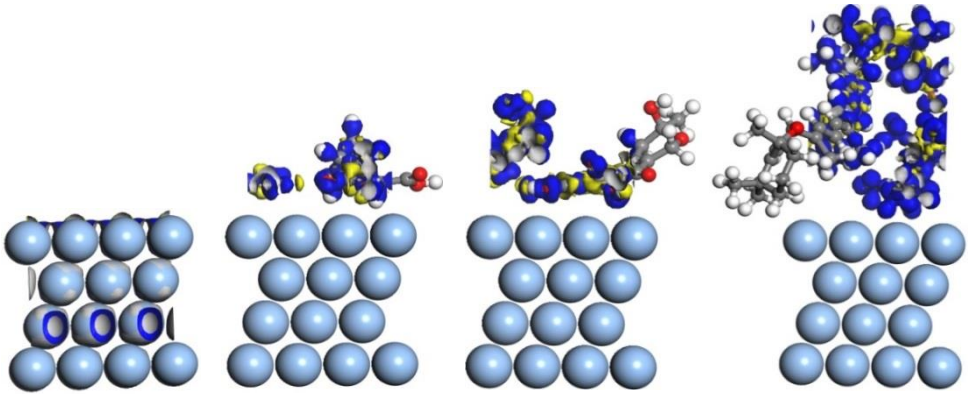
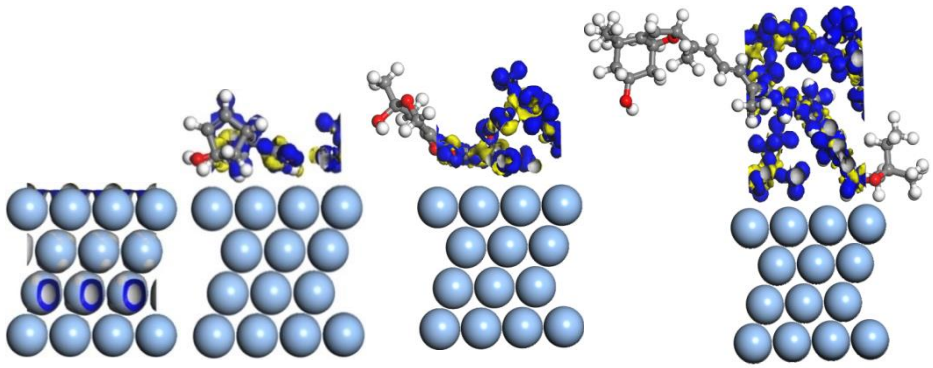


Figure B.7: Charge density difference for (a) Cry at DFT-D COSMO level of theory, (b) Cry at DFT-D gas phase level of theory. The isovalue is taken as 0.009 au.



(a) (b) (c) (d)

Figure B.8: Charge density difference for (a) Ag (111) pristine, (b) Ag (111)-HA, (c) Ag (111)-FA and (d) Ag (111)-Cry at DFT-D COSMO level of theory. The isovalue is taken as 0.009 au.



(a) (b) (c) (d)

Figure B.9: Charge density difference for (a) Ag (111) pristine, (b) Ag (111)-HA, (c) Ag (111)-FA and (d) Ag (111)-Cry at DFT-D gas phase level of theory. The isovalue is taken as 0.009 au.

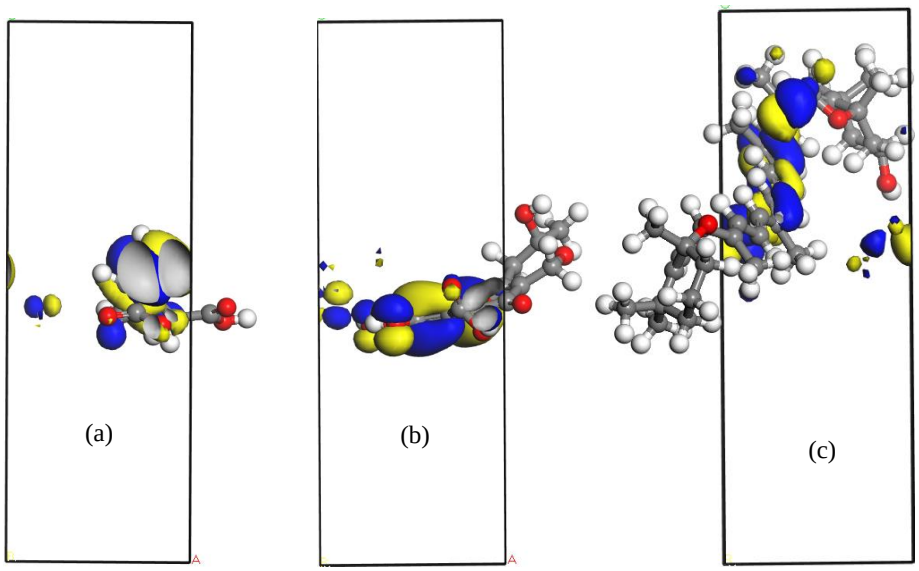


Figure B. 10: Highest Occupied Molecular Orbital for (a) HA, (b) FA (c) Cry at DFT-D COSMO level of theory. The isovalue is taken as 0.03 au.

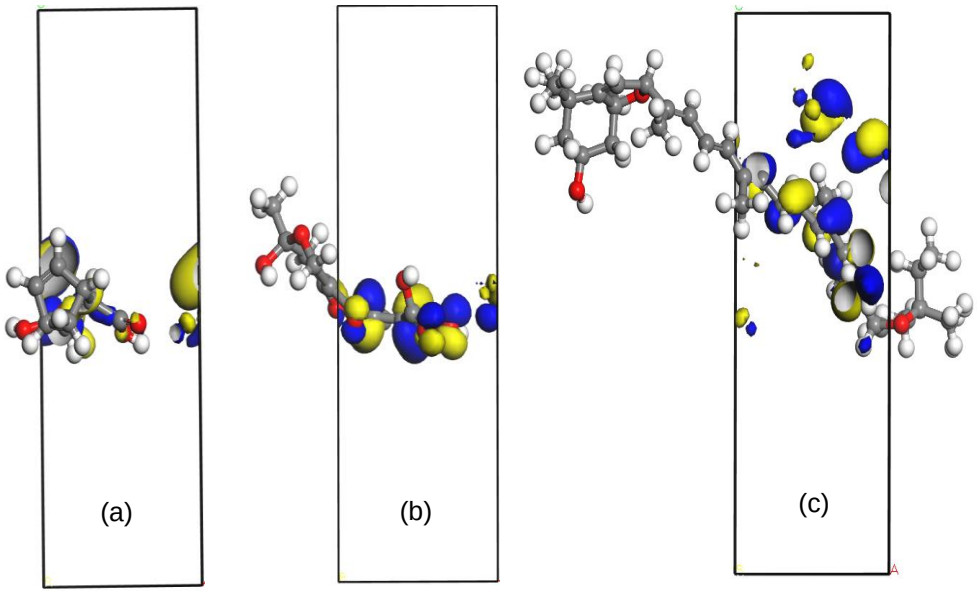


Figure B.11: Highest Occupied Molecular Orbital for (a) HA, (b) FA (c) Cry at DFT-D gas phase level of theory. The isovalue is taken as 0.03 au.

Appendix C

Adsorption and co-adsorption of natural organic matter on Ag (111) surface: A DFT-D study

Table C.1: Different configurations of Ag (111) surface when one adsorbate (formic acid) was adsorbed.

Structures	TE	Ads	RAE	DE	FA1 : dEad/dNi
Ag (1 1 1)-FA1	-36.43073973	-15.58249727	-14.88097832	-0.70151895	-15.58249727

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Formic acid (FA1).

Table C.2: Different configurations of Ag (111) surface when two adsorbates (formic acid) were adsorbed.

Structures	TE	Ads	RAE	DE	2FA1 : dEad/dNi
Ag (1 1 1)-2FA1 - 1	-85.15039517	-43.45391024	-42.28255578	-1.17135446	-28.27250439
Ag (1 1 1)-2FA1 - 2	-80.16912201	-38.47263708	-37.16788977	-1.30474732	-23.08927277
Ag (1 1 1)-2FA1 - 3	-78.51667609	-36.82019116	-35.54051387	-1.27967729	-21.34587716
Ag (1 1 1)-2FA1 - 4	-78.37456672	-36.6780818	-35.38145917	-1.29662262	-21.34002865
Ag (1 1 1)-2FA1 - 5	-76.59020235	-34.89371742	-33.56907161	-1.32464581	-19.47165208
Ag (1 1 1)-2FA1 - 6	-75.2557888	-33.55930388	-32.16092906	-1.39837482	-18.06705883
Ag (1 1 1)-2FA1 - 7	-74.87959258	-33.18310765	-31.82713003	-1.35597763	-18.00785992
Ag (1 1 1)-2FA1 - 8	-74.75168609	-33.05520117	-31.65182191	-1.40337926	-17.518448
Ag (1 1 1)-2FA1 - 9	-74.45375926	-32.75727434	-31.35420373	-1.40307061	-17.23344194
Ag (1 1 1)-2FA1 - 10	-74.24684903	-32.5503641	-31.14928082	-1.40108328	-16.98096098
Ag (1 1 1)-2FA1 - 11	-74.08832566	-32.39184073	-30.99332516	-1.39851557	-16.91980966
Ag (1 1 1)-2FA1 - 12	-73.60437013	-31.9078852	-30.5085809	-1.3993043	-16.42625807
Ag (1 1 1)-2FA1 - 13	-73.42194719	-31.72546227	-30.33162718	-1.39383509	-16.22645781
Ag (1 1 1)-2FA1 - 14	-73.14913898	-31.45265406	-30.05110376	-1.4015503	-15.9821817
Ag (1 1 1)-2FA1 - 15	-72.31222172	-30.61573679	-29.21434525	-1.40139155	-15.42643203

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Formic acid (FA1).

Table C.3: Different configurations of Ag (111) surface when three adsorbates (formic acid) were adsorbed.

Structures	TE	Ads	RAE	DE	3FA1 : dEad/dNi
Ag (1 1 1)-3FA1 - 1	-130.2521753	-67.70744794	-65.97825951	-1.72918843	-29.92391855
Ag (1 1 1)-3FA1 - 2	-126.6172052	-64.07247783	-62.22393093	-1.84854691	-20.84999754
Ag (1 1 1)-3FA1 - 3	-126.0174532	-63.47272584	-61.63330387	-1.83942197	-25.33258519
Ag (1 1 1)-3FA1 - 4	-125.727923	-63.18319563	-61.39242948	-1.79076615	-25.87234108
Ag (1 1 1)-3FA1 - 5	-125.1012339	-62.55650647	-61.07682576	-1.47968071	-25.22963022
Ag (1 1 1)-3FA1 - 6	-124.8580701	-62.31334274	-60.54725106	-1.76609169	-19.24833504
Ag (1 1 1)-3FA1 - 7	-124.51011	-61.96538256	-60.05233485	-1.91304771	-18.7994019
Ag (1 1 1)-3FA1 - 8	-124.106662	-61.56193465	-59.72377421	-1.83816044	-18.62904279
Ag (1 1 1)-3FA1 - 9	-123.7256324	-61.180905	-59.32262051	-1.85828449	-22.90633144
Ag (1 1 1)-3FA1 - 10	-123.3523864	-60.80765899	-58.98708206	-1.82057693	-22.70705674
Ag (1 1 1)-3FA1 - 11	-123.0953857	-60.55065828	-58.69528853	-1.85536974	-23.21998353
Ag (1 1 1)-3FA1 - 12	-122.8682783	-60.32355092	-58.55278548	-1.77076544	-23.06650989
Ag (1 1 1)-3FA1 - 13	-122.5246075	-59.97988005	-58.07936324	-1.90051681	-22.02007257
Ag (1 1 1)-3FA1 - 14	-122.3160859	-59.7713585	-57.85164017	-1.91971833	-22.8836492
Ag (1 1 1)-3FA1 - 15	-122.0050673	-59.46033992	-57.58728106	-1.87305886	-22.60525833
Ag (1 1 1)-3FA1 - 16	-121.7311141	-59.1863867	-57.22620384	-1.96018286	-21.12081521
Ag (1 1 1)-3FA1 - 17	-121.514156	-58.96942859	-56.98853519	-1.9808934	-20.92463465
Ag (1 1 1)-3FA1 - 18	-121.0964466	-58.55171916	-56.72477961	-1.82693955	-21.59136198
Ag (1 1 1)-3FA1 - 19	-120.5958568	-58.05112936	-56.14760173	-1.90352763	-21.73515415
Ag (1 1 1)-3FA1 - 20	-120.3422521	-57.79752466	-55.88900035	-1.9085243	-19.74311307
Ag (1 1 1)-3FA1 - 21	-120.0540902	-57.50936276	-55.59160521	-1.91775755	-21.23484436
Ag (1 1 1)-3FA1 - 22	-119.8077163	-57.26298887	-55.36546392	-1.89752495	-19.97691181
Ag (1 1 1)-3FA1 - 23	-119.5496533	-57.00492588	-54.99136229	-2.01356359	-18.81601459
Ag (1 1 1)-3FA1 - 24	-119.0963754	-56.55164801	-54.66845624	-1.88319178	-19.34434007
Ag (1 1 1)-3FA1 - 25	-118.8245405	-56.27981315	-54.28703465	-1.9927785	-19.39939316
Ag (1 1 1)-3FA1 - 26	-118.5752321	-56.03050472	-54.03721768	-1.99328703	-19.16696045

Ag (1 1 1)-3FA1 - 27	-118.3409979	-55.79627047	-53.82295871	-1.97331176	-19.51564041
Ag (1 1 1)-3FA1 - 28	-118.0253607	-55.48063332	-53.51455739	-1.96607593	-17.29553653
Ag (1 1 1)-3FA1 - 29	-117.5147901	-54.97006269	-52.97357395	-1.99648875	-18.95193871
Ag (1 1 1)-3FA1 - 30	-117.2264537	-54.68172633	-52.72992802	-1.95179831	-18.34423713
Ag (1 1 1)-3FA1 - 31	-117.0560023	-54.5112749	-52.52047849	-1.99079641	-17.0599986
Ag (1 1 1)-3FA1 - 32	-116.7614864	-54.21675898	-52.2043676	-2.01239138	-17.5265936
Ag (1 1 1)-3FA1 - 33	-116.4651537	-53.92042634	-51.9164459	-2.00398044	-17.1004602
Ag (1 1 1)-3FA1 - 34	-116.2210257	-53.67629834	-51.65530184	-2.0209965	-20.52298131
Ag (1 1 1)-3FA1 - 35	-115.9070684	-53.36234104	-51.32358481	-2.03875623	-18.60587011
Ag (1 1 1)-3FA1 - 36	-114.5029919	-51.95826455	-49.86059851	-2.09766604	-19.03927243
Ag (1 1 1)-3FA1 - 37	-114.2296163	-51.68488888	-49.60435692	-2.08053196	-18.62691408
Ag (1 1 1)-3FA1 - 38	-113.9206272	-51.37589982	-49.29327274	-2.08262708	-18.83404917
Ag (1 1 1)-3FA1 - 39	-113.6551792	-51.11045177	-49.02359727	-2.0868545	-17.73891015
Ag (1 1 1)-3FA1 - 40	-113.2800765	-50.73534908	-48.6428602	-2.09248889	-17.44736679
Ag (1 1 1)-3FA1 - 41	-112.4598576	-49.91513017	-47.84562521	-2.06950495	-17.52576281

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Formic acid (FA1).

Table C.4: Different configurations of Ag (111) surface when two adsorbates (Acetic acid) were adsorbed.

Structures	TE	Ads	RAE	DE	1AA1 : dEad/dNi
Ag (1 1 1)-1AA1	-66.45165999	-21.62940243	-20.56543483	-1.0639676	-21.62940243

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Acetic acid (AA1).

Table C.5: Different configurations of Ag (111) surface when two adsorbates (Acetic acid) were adsorbed.

Structures	TE	Ads	RAE	DE	2AA1 : dEad/dNi
Ag (1 1 1)-2AA1 - 1	-145.8416263	-56.19711124	-54.28361724	-1.913494	-34.80471549
Ag (1 1 1)-2AA1 - 2	-139.5719355	-49.92742038	-48.06124699	-1.86617338	-28.54262759
Ag (1 1 1)-2AA1 - 3	-139.2468153	-49.6023002	-47.44127284	-2.16102735	-28.24999107
Ag (1 1 1)-2AA1 - 4	-138.9708289	-49.32631376	-47.26480692	-2.06150684	-27.94672999
Ag (1 1 1)-2AA1 - 5	-138.4694042	-48.8248891	-46.79505708	-2.02983202	-27.54069159
Ag (1 1 1)-2AA1 - 6	-137.4369253	-47.79241016	-45.66966959	-2.12274057	-26.21152823
Ag (1 1 1)-2AA1 - 7	-135.8148903	-46.17037516	-44.02553313	-2.14484203	-24.777407
Ag (1 1 1)-2AA1 - 8	-135.5717252	-45.92721013	-43.75613559	-2.17107454	-24.86491756
Ag (1 1 1)-2AA1 - 9	-134.8721803	-45.22766524	-43.19643817	-2.03122707	-23.65267939
Ag (1 1 1)-2AA1 - 10	-134.63332	-44.98880486	-42.8504176	-2.13838726	-23.36846902
Ag (1 1 1)-2AA1 - 11	-134.479264	-44.83474887	-42.58506308	-2.24968579	-23.37091163
Ag (1 1 1)-2AA1 - 12	-134.0738183	-44.42930321	-42.38698054	-2.04232267	-22.85071514
Ag (1 1 1)-2AA1 - 13	-133.8684415	-44.22392644	-42.23463069	-1.98929575	-22.6739266
Ag (1 1 1)-2AA1 - 14	-133.6195224	-43.97500727	-41.67109556	-2.30391171	-22.6693264
Ag (1 1 1)-2AA1 - 15	-133.4810348	-43.83651971	-41.74757516	-2.08894455	-22.21624747
Ag (1 1 1)-2AA1 - 16	-133.0439606	-43.39944545	-40.99687964	-2.40256581	-22.51602102
Ag (1 1 1)-2AA1 - 17	-132.8066324	-43.16211731	-40.97227416	-2.18984315	-22.15771548
Ag (1 1 1)-2AA1 - 18	-132.6159681	-42.97145303	-40.89484353	-2.07660949	-21.39544984

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Acetic acid (AA1).

Table C.6: Different configurations of Ag (111) surface when three adsorbates (Acetic acid) were adsorbed.

Structures	TE	Ads	RAE	DE	3AA1 : dEad/dNi
Ag (1 1 1)-3AA1 - 1	-221.7908074	-87.32403475	-84.40858167	-2.91545308	-37.04004173
Ag (1 1 1)-3AA1 - 2	-220.1417072	-85.67493457	-82.66149221	-3.01344236	-36.62204916
Ag (1 1 1)-3AA1 - 3	-219.8454	-85.37862737	-82.71864134	-2.65998603	-36.55036209
Ag (1 1 1)-3AA1 - 4	-219.3657985	-84.89902583	-82.10883566	-2.79019017	-36.27677743
Ag (1 1 1)-3AA1 - 5	-217.8497101	-83.3829374	-80.53549952	-2.84743788	-27.6431303
Ag (1 1 1)-3AA1 - 6	-217.60905	-83.14227732	-80.30623163	-2.8360457	-27.12881817
Ag (1 1 1)-3AA1 - 7	-217.249045	-82.78227237	-79.84117485	-2.94109752	-32.40311713
Ag (1 1 1)-3AA1 - 8	-216.9114584	-82.44468577	-79.45293768	-2.99174809	-26.42488505
Ag (1 1 1)-3AA1 - 9	-216.5814278	-82.11465512	-79.14519841	-2.96945671	-26.97152755
Ag (1 1 1)-3AA1 - 10	-216.1894473	-81.72267468	-78.79082923	-2.93184545	-25.83076192
Ag (1 1 1)-3AA1 - 11	-215.7493341	-81.28256142	-78.63469832	-2.64786311	-27.06492744
Ag (1 1 1)-3AA1 - 12	-215.3845631	-80.91779048	-78.2142558	-2.70353468	-26.36007071
Ag (1 1 1)-3AA1 - 13	-214.7915663	-80.32479367	-77.48851354	-2.83628013	-30.60724635
Ag (1 1 1)-3AA1 - 14	-214.3615057	-79.89473304	-76.9944966	-2.90023643	-23.81054349
Ag (1 1 1)-3AA1 - 15	-214.1447729	-79.67800026	-76.69741037	-2.9805899	-23.64423255
Ag (1 1 1)-3AA1 - 16	-213.8297543	-79.36298163	-76.39020769	-2.97277394	-23.22671846
Ag (1 1 1)-3AA1 - 17	-213.4786297	-79.01185705	-76.39839977	-2.61345728	-28.94698551
Ag (1 1 1)-3AA1 - 18	-213.1753953	-78.70862264	-75.93187258	-2.77675006	-23.99281536
Ag (1 1 1)-3AA1 - 19	-212.9610962	-78.49432355	-75.33961345	-3.1547101	-29.0694917
Ag (1 1 1)-3AA1 - 20	-212.7403463	-78.27357362	-75.33743089	-2.93614273	-29.00231421
Ag (1 1 1)-3AA1 - 21	-212.5108367	-78.04406405	-75.17360539	-2.87045866	-28.36616634
Ag (1 1 1)-3AA1 - 22	-212.2696209	-77.80284828	-74.78443538	-3.0184129	-28.00335572
Ag (1 1 1)-3AA1 - 23	-212.0324909	-77.56571821	-74.36841313	-3.19730508	-28.51844946
Ag (1 1 1)-3AA1 - 24	-211.371261	-76.9044883	-73.64734599	-3.25714231	-27.56422845
Ag (1 1 1)-3AA1 - 25	-211.0352781	-76.56850544	-73.56882451	-2.99968094	-27.46755735
Ag (1 1 1)-3AA1 - 26	-210.8350908	-76.36831819	-73.4037513	-2.96456689	-27.87834923

Ag (1 1 1)-3AA1 - 27	-210.5317326	-76.06495999	-73.00349351	-3.06146648	-26.79038658
Ag (1 1 1)-3AA1 - 28	-210.2565561	-75.78978342	-73.07312289	-2.71666054	-26.23111916
Ag (1 1 1)-3AA1 - 29	-210.0092136	-75.54244096	-72.61907232	-2.92336864	-26.54459018
Ag (1 1 1)-3AA1 - 30	-209.4895345	-75.02276183	-72.08680853	-2.9359533	-25.76212337
Ag (1 1 1)-3AA1 - 31	-209.1225638	-74.65579112	-71.49194915	-3.16384197	-27.0823211
Ag (1 1 1)-3AA1 - 32	-208.6639347	-74.19716203	-71.48250747	-2.71465455	-24.61411625
Ag (1 1 1)-3AA1 - 33	-208.1070211	-73.64024849	-70.54254241	-3.09770608	-26.15019779
Ag (1 1 1)-3AA1 - 34	-207.3863188	-72.91954616	-69.59098546	-3.3285607	-23.8585994
Ag (1 1 1)-3AA1 - 35	-207.0693551	-72.60258241	-70.00529932	-2.59728309	-27.36558792
Ag (1 1 1)-3AA1 - 36	-206.7904766	-72.32370395	-69.22544495	-3.098259	-26.29143739
Ag (1 1 1)-3AA1 - 37	-206.5724812	-72.10570857	-68.80299607	-3.30271251	-24.15823298
Ag (1 1 1)-3AA1 - 38	-206.0555057	-71.58873304	-68.78308185	-2.80565119	-25.40809047
Ag (1 1 1)-3AA1 - 39	-205.7251602	-71.25838752	-68.97104913	-2.28733839	-27.25480387
Ag (1 1 1)-3AA1 - 40	-205.4022637	-70.93549101	-67.85372019	-3.08177082	-22.15248882
Ag (1 1 1)-3AA1 - 41	-205.1005641	-70.63379148	-67.68486989	-2.94892159	-24.90323887
Ag (1 1 1)-3AA1 - 42	-203.3839971	-68.91722448	-65.78348762	-3.13373685	-19.08006089
Ag (1 1 1)-3AA1 - 43	-202.9971077	-68.53033503	-65.32595425	-3.20438078	-19.13344625
Ag (1 1 1)-3AA1 - 44	-202.332269	-67.8654963	-64.69890106	-3.16659523	-23.03751966
Ag (1 1 1)-3AA1 - 45	-201.3662926	-66.89951998	-63.68382132	-3.21569866	-23.10891542

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Acetic acid (AA1).

Table C.7: Different configurations of Ag (111) surface when one adsorbate (Ascorbic acid) were adsorbed.

Structures	TE	Ads	RAE	DE	1AA2 : dEad/dNi
Ag (1 1 1)-1AA2 - 1	-22.2082068	-60.84734683	-41.57110666	-19.27624017	-60.84734683
Ag (1 1 1)-1AA2 - 2	-21.749431	-60.38857109	-41.77226236	-18.61630873	-60.38857109
Ag (1 1 1)-1AA2 - 3	-21.2160637	-59.85520372	-41.33070257	-18.52450114	-59.85520372
Ag (1 1 1)-1AA2 - 4	-20.2880904	-58.92723041	-40.9018006	-18.02542981	-58.92723041

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Ascorbic acid (AA2).

Table C.8: Different configurations of Ag (111) surface when two adsorbates (Ascorbic acid) were adsorbed.

Structures	TE	Ads	RAE	DE	2AA2 : dEad/dNi
Ag (1 1 1)-2AA2 - 1	-62.5096641	-139.7879442	-109.9328524	-29.85509175	-82.68451831
Ag (1 1 1)-2AA2 - 2	-62.1584188	-139.4366989	-111.0405698	-28.39612916	-81.6440153
Ag (1 1 1)-2AA2 - 3	-61.705557	-138.9838372	-105.8133829	-33.17045425	-79.65738152
Ag (1 1 1)-2AA2 - 4	-60.0732239	-137.351504	-110.1034192	-27.24808478	-81.38004045
Ag (1 1 1)-2AA2 - 5	-59.617906	-136.8961861	-114.1693761	-22.72681004	-83.33239378
Ag (1 1 1)-2AA2 - 6	-59.1653874	-136.4436675	-110.9182206	-25.52544694	-83.12844981
Ag (1 1 1)-2AA2 - 7	-58.0024269	-135.280707	-104.5596931	-30.72101392	-79.32816119
Ag (1 1 1)-2AA2 - 8	-57.5378153	-134.8160954	-112.3338029	-22.48229252	-82.14276329
Ag (1 1 1)-2AA2 - 9	-57.2572053	-134.5354854	-109.7631182	-24.77236722	-82.62053053
Ag (1 1 1)-2AA2 - 10	-57.0300075	-134.3082877	-106.2606517	-28.04763593	-75.0573025
Ag (1 1 1)-2AA2 - 11	-56.7337752	-134.0120553	-99.51380903	-34.49824631	-75.56343222
Ag (1 1 1)-2AA2 - 12	-56.3127147	-133.5909948	-106.3907956	-27.20019924	-76.17443143
Ag (1 1 1)-2AA2 - 13	-56.0927963	-133.3710765	-107.9833972	-25.38767928	-80.7927747
Ag (1 1 1)-2AA2 - 14	-55.857624	-133.1359041	-107.502146	-25.63375809	-78.82877466
Ag (1 1 1)-2AA2 - 15	-55.6225937	-132.9008738	-104.4843337	-28.41654015	-73.11151739
Ag (1 1 1)-2AA2 - 16	-55.3286489	-132.6069291	-105.1973296	-27.40959943	-76.39447669
Ag (1 1 1)-2AA2 - 17	-55.082456	-132.3607361	-109.3916005	-22.96913566	-77.04718392
Ag (1 1 1)-2AA2 - 18	-54.7884444	-132.0667245	-107.7188306	-24.34789397	-79.64777622
Ag (1 1 1)-2AA2 - 19	-54.4359156	-131.7141958	-104.1153609	-27.59883485	-77.14449394
Ag (1 1 1)-2AA2 - 20	-54.1278824	-131.4061626	-103.6303136	-27.77584894	-77.43884876
Ag (1 1 1)-2AA2 - 21	-53.9254478	-131.203728	-110.7832128	-20.4205152	-78.50210988
Ag (1 1 1)-2AA2 - 22	-53.5682004	-130.8464806	-103.5457867	-27.30069386	-77.17968422
Ag (1 1 1)-2AA2 - 23	-53.294362	-130.5726421	-104.1032601	-26.46938202	-76.55844766
Ag (1 1 1)-2AA2 - 24	-53.0920293	-130.3703094	-100.0452629	-30.32504648	-73.57073635
Ag (1 1 1)-2AA2 - 25	-52.7621498	-130.04043	-103.0531759	-26.98725403	-71.90453091
Ag (1 1 1)-2AA2 - 26	-52.3503946	-129.6286747	-102.3685601	-27.26011459	-75.84614308

Ag (1 1 1)-2AA2 - 27	-52.0578259	-129.336106	-102.7634434	-26.57266265	-74.30878421
Ag (1 1 1)-2AA2 - 28	-51.856534	-129.1348141	-98.89124343	-30.24357064	-71.65279543
Ag (1 1 1)-2AA2 - 29	-51.3142494	-128.5925295	-101.6379131	-26.95461642	-73.42119631
Ag (1 1 1)-2AA2 - 30	-50.9488346	-128.2271147	-104.3754031	-23.85171159	-76.48656446
Ag (1 1 1)-2AA2 - 31	-50.7331536	-128.0114338	-101.1245855	-26.88684826	-74.230113
Ag (1 1 1)-2AA2 - 32	-50.4464436	-127.7247237	-99.3797753	-28.34494837	-73.64955947
Ag (1 1 1)-2AA2 - 33	-50.245102	-127.5233821	-98.94999002	-28.57339204	-72.71367962
Ag (1 1 1)-2AA2 - 34	-49.986322	-127.2646021	-100.5998212	-26.66478084	-67.94756418
Ag (1 1 1)-2AA2 - 35	-49.5911291	-126.8694092	-97.27820363	-29.5912056	-73.07538903
Ag (1 1 1)-2AA2 - 36	-49.197806	-126.4760861	-102.3394477	-24.13663842	-71.70170921
Ag (1 1 1)-2AA2 - 37	-48.9965347	-126.2748148	-95.30597282	-30.96884201	-69.33266348
Ag (1 1 1)-2AA2 - 38	-48.7710407	-126.0493208	-94.47377619	-31.57554465	-70.48166208
Ag (1 1 1)-2AA2 - 39	-48.4795008	-125.7577809	-106.5460202	-19.21176076	-73.45616384
Ag (1 1 1)-2AA2 - 40	-48.2324227	-125.5107028	-97.66973377	-27.840969	-67.30897921
Ag (1 1 1)-2AA2 - 41	-47.8404197	-125.1186998	-95.31100844	-29.80769132	-68.53983251
Ag (1 1 1)-2AA2 - 42	-47.6257797	-124.9040598	-103.2079354	-21.6961244	-74.64401779
Ag (1 1 1)-2AA2 - 43	-47.365954	-124.6442341	-94.36485186	-30.27938222	-67.15122554
Ag (1 1 1)-2AA2 - 44	-46.9984776	-124.2767577	-102.9958895	-21.28086822	-73.19388989
Ag (1 1 1)-2AA2 - 45	-46.7364435	-124.0147236	-95.76202037	-28.25270327	-70.7305619
Ag (1 1 1)-2AA2 - 46	-46.403456	-123.6817361	-95.70249776	-27.97923834	-65.29613183
Ag (1 1 1)-2AA2 - 47	-45.8016913	-123.0799714	-98.69693832	-24.38303307	-70.83551583
Ag (1 1 1)-2AA2 - 48	-45.5535612	-122.8318413	-94.10010263	-28.73173871	-66.23330192
Ag (1 1 1)-2AA2 - 49	-45.2027492	-122.4810293	-96.47872031	-26.00230899	-69.642692
Ag (1 1 1)-2AA2 - 50	-44.6275352	-121.9058153	-94.1734379	-27.73237737	-65.4754311
Ag (1 1 1)-2AA2 - 51	-43.5640386	-120.8423187	-99.35988693	-21.48243179	-71.6334882
Ag (1 1 1)-2AA2 - 52	-43.0552474	-120.3335275	-95.9347636	-24.39876388	-68.94956018
Ag (1 1 1)-2AA2 - 53	-40.2856366	-117.5639167	-96.2015342	-21.36238247	-69.47646884

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Ascorbic acid (AA2).

Table C.9: Different configurations of Ag (111) surface when three adsorbates (Ascorbic acid) were adsorbed.

Structures	TE	Ads	RAE	DE	3AA2 : dEad/dNi
Ag (1 1 1)-3AA2 - 1	-63.0288224	-140.3071025	-111.6240523	-28.68305023	-84.37932136
Ag (1 1 1)-3AA2 - 2	-62.8143458	-140.0926259	-108.5738666	-31.51875928	-83.13404589
Ag (1 1 1)-3AA2 - 3	-62.3642651	-139.6425453	-112.8521801	-26.79036511	-82.88991889
Ag (1 1 1)-3AA2 - 4	-61.9289338	-139.2072139	-106.2713432	-32.93587064	-81.24099671
Ag (1 1 1)-3AA2 - 5	-61.7057456	-138.9840257	-105.806795	-33.1772307	-79.65484326
Ag (1 1 1)-3AA2 - 6	-60.4220809	-137.7003611	-110.4175275	-27.28283353	-82.22180311
Ag (1 1 1)-3AA2 - 7	-60.2173959	-137.495676	-105.6728707	-31.82280534	-79.19899979
Ag (1 1 1)-3AA2 - 8	-59.6938197	-136.9720998	-110.0014722	-26.9706276	-83.11285007
Ag (1 1 1)-3AA2 - 9	-59.4280738	-136.7063539	-107.9655775	-28.74077642	-81.75919284
Ag (1 1 1)-3AA2 - 10	-59.0975165	-136.3757966	-103.426463	-32.9493336	-80.63936558
Ag (1 1 1)-3AA2 - 11	-58.7263323	-136.0046124	-103.1762281	-32.82838436	-77.66554786
Ag (1 1 1)-3AA2 - 12	-58.4824866	-135.7607667	-101.9840342	-33.77673252	-79.22745056
Ag (1 1 1)-3AA2 - 13	-58.1214542	-135.3997343	-102.7429385	-32.65679582	-79.64105509
Ag (1 1 1)-3AA2 - 14	-57.9156652	-135.1939453	-106.8321379	-28.3618074	-78.44378311
Ag (1 1 1)-3AA2 - 15	-57.5762577	-134.8545378	-106.1966308	-28.65790697	-78.87051412
Ag (1 1 1)-3AA2 - 16	-57.3062883	-134.5845684	-102.6002564	-31.98431206	-77.50444636
Ag (1 1 1)-3AA2 - 17	-57.0482449	-134.326525	-102.0563778	-32.27014726	-78.80889299
Ag (1 1 1)-3AA2 - 18	-56.6977004	-133.9759805	-103.7197454	-30.25623513	-75.41207376
Ag (1 1 1)-3AA2 - 19	-56.388502	-133.6667821	-99.89480388	-33.77197822	-77.78149846
Ag (1 1 1)-3AA2 - 20	-56.1596685	-133.4379486	-108.6539434	-24.78400518	-80.05041533
Ag (1 1 1)-3AA2 - 21	-55.6646589	-132.942939	-104.2113536	-28.73158538	-77.02258748
Ag (1 1 1)-3AA2 - 22	-55.379244	-132.6575242	-101.7267017	-30.93082242	-76.1354825
Ag (1 1 1)-3AA2 - 23	-55.0708858	-132.3491659	-109.8644056	-22.48476031	-77.3351467
Ag (1 1 1)-3AA2 - 24	-54.8569361	-132.1352162	-110.7076993	-21.42751688	-76.59552852
Ag (1 1 1)-3AA2 - 25	-54.520319	-131.7985991	-101.9482637	-29.85033535	-76.97047413
Ag (1 1 1)-3AA2 - 26	-54.1614488	-131.4397289	-99.78440486	-31.65532407	-73.32793279

Ag (1 1 1)-3AA2 - 27	-53.9250342	-131.2033143	-110.7912774	-20.41203685	-78.50595831
Ag (1 1 1)-3AA2 - 28	-53.4890127	-130.7672928	-103.4016635	-27.36562934	-73.57176669
Ag (1 1 1)-3AA2 - 29	-53.1388973	-130.4171774	-109.444878	-20.97229939	-76.62807553
Ag (1 1 1)-3AA2 - 30	-52.905354	-130.1836341	-101.1295466	-29.05408753	-72.6105007
Ag (1 1 1)-3AA2 - 31	-52.6959449	-129.974225	-97.65079408	-32.32343093	-70.31634468
Ag (1 1 1)-3AA2 - 32	-52.3931353	-129.6714155	-92.47828465	-37.1931308	-72.4725165
Ag (1 1 1)-3AA2 - 33	-52.014231	-129.2925112	-98.27967973	-31.01283142	-71.3368995
Ag (1 1 1)-3AA2 - 34	-51.6226825	-128.9009627	-105.8220855	-23.07887717	-76.19486201
Ag (1 1 1)-3AA2 - 35	-51.0135717	-128.2918518	-98.28400035	-30.00785145	-70.58430391
Ag (1 1 1)-3AA2 - 36	-50.7634737	-128.0417538	-105.9173083	-22.12444549	-71.88991167
Ag (1 1 1)-3AA2 - 37	-50.4068755	-127.6851556	-95.49099245	-32.19416313	-74.06065456
Ag (1 1 1)-3AA2 - 38	-49.9484866	-127.2267667	-96.3880021	-30.83876456	-71.04446767
Ag (1 1 1)-3AA2 - 39	-49.3384766	-126.6167568	-105.0192567	-21.59750002	-73.08593765
Ag (1 1 1)-3AA2 - 40	-49.1014692	-126.3797493	-96.74853649	-29.63121277	-73.30731853
Ag (1 1 1)-3AA2 - 41	-48.819708	-126.0979881	-95.80081204	-30.29717603	-66.99711113
Ag (1 1 1)-3AA2 - 42	-48.5832202	-125.8615003	-95.22509715	-30.63640314	-69.45042899
Ag (1 1 1)-3AA2 - 43	-48.222726	-125.5010061	-98.39688222	-27.10412387	-71.57050616
Ag (1 1 1)-3AA2 - 44	-47.8403905	-125.1186706	-95.3112056	-29.80746498	-68.53992961
Ag (1 1 1)-3AA2 - 45	-47.6255076	-124.9037877	-101.7333948	-23.17039293	-74.5646871
Ag (1 1 1)-3AA2 - 46	-47.3791141	-124.6573942	-93.8848188	-30.77257543	-72.77249081
Ag (1 1 1)-3AA2 - 47	-46.5577738	-123.836054	-95.99621734	-27.83983662	-65.19846536
Ag (1 1 1)-3AA2 - 48	-45.9245125	-123.2027926	-96.15058015	-27.05221243	-70.043895
Ag (1 1 1)-3AA2 - 49	-45.4265039	-122.704784	-96.53341063	-26.1713734	-71.5488499
Ag (1 1 1)-3AA2 - 50	-44.8855439	-122.1638241	-91.58062503	-30.58319903	-62.0849944
Ag (1 1 1)-3AA2 - 51	-43.8828155	-121.1610957	-99.71513859	-21.44595706	-75.86100117
Ag (1 1 1)-3AA2 - 52	-43.5639687	-120.8422488	-99.36035653	-21.48189231	-71.63289715
Ag (1 1 1)-3AA2 - 53	-38.579237	-115.8575171	-93.22528361	-22.63223347	-68.99885458

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Ascorbic acid (AA2).

Table C.10: Different configurations of Ag (111) surface when one formic acid (FAI) and one acetic acid (AA1) adsorbates were adsorbed.

Structures	TE	Ads	RAE	DE	1AA1 : dEad/dNi	1FA1: dEad/dNi
Ag (1 1 1)-1AA1,1FA1 - 1	-191.2297733	-80.7370157	-78.27863894	-2.45837676	-36.7177193	-30.48793123
Ag (1 1 1)-1AA1,1FA1 - 2	-189.7285646	-79.23580706	-76.68538324	-2.55042382	-35.79302604	-30.23835134
Ag (1 1 1)-1AA1,1FA1 - 3	-187.1176842	-76.6249266	-74.14298123	-2.48194537	-27.21756035	-27.49640269
Ag (1 1 1)-1AA1,1FA1 - 4	-186.8973146	-76.40455707	-73.88082868	-2.52372839	-32.9863906	-28.97835276
Ag (1 1 1)-1AA1,1FA1 - 5	-186.6550505	-76.16229295	-73.63011733	-2.53217562	-34.40023599	-25.8792647
Ag (1 1 1)-1AA1,1FA1 - 6	-186.4540708	-75.96131319	-73.39781415	-2.56349904	-31.98394201	-29.78588267
Ag (1 1 1)-1AA1,1FA1 - 7	-186.1285863	-75.63582876	-73.08932148	-2.54650728	-36.12194015	-20.61718852
Ag (1 1 1)-1AA1,1FA1 - 8	-185.8663275	-75.37356997	-72.74397599	-2.62959398	-26.21330515	-30.8462495
Ag (1 1 1)-1AA1,1FA1 - 9	-185.5899124	-75.09715487	-72.9102995	-2.18685537	-32.41701593	-26.09602449
Ag (1 1 1)-1AA1,1FA1 - 10	-185.3123529	-74.81959537	-72.28462996	-2.53496541	-26.03292123	-32.96738203
Ag (1 1 1)-1AA1,1FA1 - 11	-184.9716245	-74.4788669	-71.78891657	-2.68995033	-29.80965812	-24.94873196
Ag (1 1 1)-1AA1,1FA1 - 12	-184.6995555	-74.20679789	-71.7928592	-2.41393869	-30.00159102	-25.02734039
Ag (1 1 1)-1AA1,1FA1 - 13	-184.3088455	-73.81608792	-71.26839176	-2.54769616	-35.70464863	-17.76095268
Ag (1 1 1)-1AA1,1FA1 - 14	-184.0189384	-73.52618084	-70.92072971	-2.60545113	-33.8526499	-17.38665172
Ag (1 1 1)-1AA1,1FA1 - 15	-183.7286024	-73.23584485	-70.73473845	-2.50110639	-34.86395398	-18.28688469
Ag (1 1 1)-1AA1,1FA1 - 16	-183.4954898	-73.00273219	-70.43134778	-2.57138441	-29.88548883	-23.49480059
Ag (1 1 1)-1AA1,1FA1 - 17	-183.2651347	-72.77237714	-70.24543557	-2.52694157	-23.1676541	-28.17176313
Ag (1 1 1)-1AA1,1FA1 - 18	-183.0357473	-72.54298973	-69.95944242	-2.58354731	-23.9257064	-29.5108736
Ag (1 1 1)-1AA1,1FA1 - 19	-182.7598413	-72.26708375	-69.57887342	-2.68821033	-22.56632377	-28.72195804
Ag (1 1 1)-1AA1,1FA1 - 20	-182.5284032	-72.03564565	-69.4549007	-2.58074495	-28.61944987	-23.9338774
Ag (1 1 1)-1AA1,1FA1 - 21	-182.278339	-71.78558146	-69.16329519	-2.62228627	-29.78139058	-22.83336928
Ag (1 1 1)-1AA1,1FA1 - 22	-182.0125656	-71.51980805	-68.76051093	-2.75929712	-28.08830315	-24.49414211
Ag (1 1 1)-1AA1,1FA1 - 23	-181.7605869	-71.26782932	-68.82636768	-2.44146164	-29.10435828	-21.80988955
Ag (1 1 1)-1AA1,1FA1 - 24	-181.311481	-70.81872342	-68.51436001	-2.30436341	-27.51137956	-24.17507391
Ag (1 1 1)-1AA1,1FA1 - 25	-181.1058805	-70.61312294	-67.912534	-2.70058894	-27.70515973	-25.09639583
Ag (1 1 1)-1AA1,1FA1 - 26	-180.8186892	-70.32593163	-67.64462386	-2.68130777	-26.72946715	-23.72368015

Ag (1 1 1)-1AA1,1FA1 - 27	-180.3969685	-69.90421098	-67.42037264	-2.48383834	-27.60844138	-25.74086484
Ag (1 1 1)-1AA1,1FA1 - 28	-180.0117394	-69.51898179	-66.91830143	-2.60068036	-26.70613782	-25.23061516
Ag (1 1 1)-1AA1,1FA1 - 29	-179.7665526	-69.27379502	-66.57065681	-2.70313821	-29.8068019	-19.71640113
Ag (1 1 1)-1AA1,1FA1 - 30	-179.401821	-68.90906344	-66.02838816	-2.88067529	-27.94261897	-22.10962708
Ag (1 1 1)-1AA1,1FA1 - 31	-179.1680899	-68.67533236	-65.96423165	-2.71110071	-25.99945004	-22.83378788
Ag (1 1 1)-1AA1,1FA1 - 32	-178.7807718	-68.28801423	-65.55466408	-2.73335015	-29.98463438	-18.69655775
Ag (1 1 1)-1AA1,1FA1 - 33	-178.4713309	-67.97857335	-65.17057006	-2.80800329	-28.30818703	-20.39418678
Ag (1 1 1)-1AA1,1FA1 - 34	-178.2349356	-67.74217804	-65.1241206	-2.61805744	-29.85830704	-18.95587129
Ag (1 1 1)-1AA1,1FA1 - 35	-178.01892	-67.5261624	-64.63932541	-2.88683699	-26.43680471	-24.48156847
Ag (1 1 1)-1AA1,1FA1 - 36	-177.6223639	-67.1296063	-64.37971148	-2.74989482	-23.85574385	-22.22735989
Ag (1 1 1)-1AA1,1FA1 - 37	-177.3620266	-66.86926907	-64.11049348	-2.75877559	-28.37764382	-18.11285582
Ag (1 1 1)-1AA1,1FA1 - 38	-177.061816	-66.56905847	-63.78924867	-2.7798098	-22.90942233	-23.52934912
Ag (1 1 1)-1AA1,1FA1 - 39	-176.6261173	-66.1333597	-63.49671176	-2.63664794	-25.3888663	-20.4606011
Ag (1 1 1)-1AA1,1FA1 - 40	-176.006643	-65.51388543	-62.67375431	-2.84013111	-26.38223882	-20.19323664
Ag (1 1 1)-1AA1,1FA1 - 41	-175.7754688	-65.28271123	-62.5434187	-2.73929253	-25.99325884	-19.56716637
Ag (1 1 1)-1AA1,1FA1 - 42	-175.3900677	-64.8973101	-62.29770836	-2.59960174	-23.80551663	-21.31260265
Ag (1 1 1)-1AA1,1FA1 - 43	-174.497943	-64.00518538	-61.27710956	-2.72807582	-25.41081984	-18.87785759
Ag (1 1 1)-1AA1,1FA1 - 44	-173.4074237	-62.91466612	-59.98640288	-2.92826324	-24.52525284	-18.35593979

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Acetic acid (AA1), Formic acid (FA1).

Table C.11: Different configurations of Ag (111) surface when one formic acid (FAI) and one ascorbic acid (AA2) adsorbates were adsorbed.

Structures	TE	Ads	RAE	DE	1AA2 : dEad/dNi	1FA1: dEad/dNi
Ag (1 1 1)-1AA2,1FA1 – 1	-71.53545927	-89.32635687	-69.70644398	-19.61991289	-75.04501388	-31.57801514
Ag (1 1 1)-1AA2,1FA1 – 2	-71.31021097	-89.10110856	-69.65580036	-19.4453082	-74.01829925	-30.34350956
Ag (1 1 1)-1AA2,1FA1 – 3	-70.79278254	-88.58368013	-69.67978823	-18.9038919	-73.55702833	-28.8930777
Ag (1 1 1)-1AA2,1FA1 – 4	-70.17722955	-87.96812715	-69.64410454	-18.3240226	-73.1022393	-28.94120493

Ag (1 1 1)-1AA2,1FA1 – 5	-69.87259267	-87.66349026	-69.11290657	-18.55058369	-72.93778361	-28.34928835
Ag (1 1 1)-1AA2,1FA1 – 6	-69.46668703	-87.25758463	-69.62816692	-17.6294177	-72.98622826	-27.73569866
Ag (1 1 1)-1AA2,1FA1 – 7	-69.15913562	-86.95003321	-70.12509846	-16.82493475	-72.00990797	-27.84786329
Ag (1 1 1)-1AA2,1FA1 – 8	-68.83952471	-86.6304223	-73.68173349	-12.94868881	-71.93802038	-30.39812744
Ag (1 1 1)-1AA2,1FA1 – 9	-68.3054343	-86.09633189	-66.93850651	-19.15782538	-71.15656103	-28.76495833
Ag (1 1 1)-1AA2,1FA1 – 10	-67.93161418	-85.72251178	-67.24159223	-18.48091954	-71.16129571	-26.04769286
Ag (1 1 1)-1AA2,1FA1 – 11	-67.66119636	-85.45209396	-66.77097253	-18.68112143	-71.81825606	-28.78651224
Ag (1 1 1)-1AA2,1FA1 – 12	-67.16318929	-84.95408689	-69.15113351	-15.80295338	-70.14162052	-28.05340463
Ag (1 1 1)-1AA2,1FA1 – 13	-66.95296394	-84.74386154	-68.73327591	-16.01058563	-70.5312798	-26.71923128
Ag (1 1 1)-1AA2,1FA1 – 14	-66.41368499	-84.20458259	-75.14881872	-9.05576387	-69.62579351	-32.3922959
Ag (1 1 1)-1AA2,1FA1 – 15	-66.34723931	-84.1381369	-64.18688102	-19.95125588	-68.82814961	-23.62268934
Ag (1 1 1)-1AA2,1FA1 – 16	-66.11114331	-83.90204091	-64.7585209	-19.14352001	-68.8942469	-24.57536731
Ag (1 1 1)-1AA2,1FA1 – 17	-65.83116193	-83.62205952	-69.76112438	-13.86093514	-69.37001204	-28.33157381
Ag (1 1 1)-1AA2,1FA1 – 18	-65.53035764	-83.32125523	-64.72157822	-18.599677	-68.20781105	-23.98902922
Ag (1 1 1)-1AA2,1FA1 – 19	-65.1722408	-82.96313839	-65.13757751	-17.82556088	-67.72836927	-24.81841098
Ag (1 1 1)-1AA2,1FA1 – 20	-64.90615668	-82.69705428	-63.6959321	-19.00112218	-67.42380168	-22.92246369
Ag (1 1 1)-1AA2,1FA1 – 21	-64.68723295	-82.47813054	-68.85940983	-13.61872071	-67.75617039	-26.78906983
Ag (1 1 1)-1AA2,1FA1 – 22	-64.4784032	-82.2693008	-67.62921477	-14.64008603	-68.643404	-27.21433858
Ag (1 1 1)-1AA2,1FA1 – 23	-64.12066934	-81.91156693	-62.48328209	-19.42828484	-66.89137019	-23.13555189
Ag (1 1 1)-1AA2,1FA1 – 24	-63.8697434	-81.66064099	-62.17210299	-19.488538	-66.61039625	-22.19263902
Ag (1 1 1)-1AA2,1FA1 – 25	-63.53339361	-81.32429121	-64.98507628	-16.33921493	-67.78758792	-23.52250724
Ag (1 1 1)-1AA2,1FA1 – 26	-63.23357459	-81.02447218	-66.79524182	-14.22923037	-65.7180956	-25.29451585
Ag (1 1 1)-1AA2,1FA1 – 27	-62.91130739	-80.70220498	-61.75471779	-18.94748719	-66.54392989	-20.6453997
Ag (1 1 1)-1AA2,1FA1 – 28	-62.03084301	-79.8217406	-65.9027595	-13.9189811	-65.08428791	-25.0182614
Ag (1 1 1)-1AA2,1FA1 – 29	-61.19720271	-78.9881003	-64.63131099	-14.35678932	-67.08791057	-23.89062308
Ag (1 1 1)-1AA2,1FA1 – 30	-60.4267553	-78.21765289	-64.06107674	-14.15657615	-64.55063321	-23.70753947
Ag (1 1 1)-1AA2,1FA1 – 31	-58.76095076	-76.55184835	-61.5400513	-15.01179705	-63.02687327	-21.44669947
Ag (1 1 1)-1AA2,1FA1 – 32	-55.29703648	-73.08793407	-59.5789369	-13.50899717	-58.73708731	-20.45908273

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Ascorbic acid (AA2),Formic acid (FA1).

Table C.12: Different configurations of Ag (111) surface when one acetic acid (AAI) and one ascorbic acid (AA2) adsorbates were adsorbed.

Structures	TE	Ads	RAE	DE	1AA2 : dEad/dNi	1AA1: dEad/dNi
Ag (1 1 1)-1AA1,1AA2 - 1	-102.4117464	-96.22862891	-76.27854738	-19.95008153	-75.76497614	-38.39951075
Ag (1 1 1)-1AA1,1AA2 - 2	-102.1425498	-95.95943234	-76.25554681	-19.70388553	-75.15404221	-36.2981582
Ag (1 1 1)-1AA1,1AA2 - 3	-101.7499427	-95.56682525	-77.35646329	-18.21036196	-75.54964671	-37.82083907
Ag (1 1 1)-1AA1,1AA2 - 4	-100.4737281	-94.29061058	-74.17688898	-20.1137216	-73.77038506	-35.40240149
Ag (1 1 1)-1AA1,1AA2 - 5	-100.114199	-93.93108145	-76.37491633	-17.55616512	-72.84567629	-35.08252982
Ag (1 1 1)-1AA1,1AA2 - 6	-99.76785205	-93.58473456	-75.17508191	-18.40965265	-73.25267681	-34.95320167
Ag (1 1 1)-1AA1,1AA2 - 7	-99.47353172	-93.29041422	-76.64094671	-16.64946751	-72.2224141	-35.29550426
Ag (1 1 1)-1AA1,1AA2 - 8	-99.18814198	-93.00502449	-76.00089887	-17.00412562	-72.99379169	-34.13263252
Ag (1 1 1)-1AA1,1AA2 - 9	-98.87212221	-92.68900472	-73.79252092	-18.8964838	-71.42921106	-35.12697972
Ag (1 1 1)-1AA1,1AA2 - 10	-98.6668205	-92.48370301	-78.07044636	-14.41325665	-71.27998875	-36.68411701
Ag (1 1 1)-1AA1,1AA2 - 11	-98.38662951	-92.20351202	-81.71524787	-10.48826414	-72.70857907	-39.39520568
Ag (1 1 1)-1AA1,1AA2 - 12	-98.07626268	-91.89314519	-74.56824659	-17.3248986	-72.36498196	-34.03889756
Ag (1 1 1)-1AA1,1AA2 - 13	-97.61810355	-91.43498605	-71.24402106	-20.190965	-70.17851012	-30.81226816
Ag (1 1 1)-1AA1,1AA2 - 14	-97.49007124	-91.30695374	-74.82120629	-16.48574745	-71.68189327	-34.02479262
Ag (1 1 1)-1AA1,1AA2 - 15	-96.74544046	-90.56232296	-74.35973722	-16.20258574	-69.99242957	-34.29155896
Ag (1 1 1)-1AA1,1AA2 - 16	-96.43492773	-90.25181024	-71.68470659	-18.56710365	-70.35389264	-30.98149963
Ag (1 1 1)-1AA1,1AA2 - 17	-96.18801968	-90.00490219	-73.76783486	-16.23706733	-69.88710864	-33.34465021
Ag (1 1 1)-1AA1,1AA2 - 18	-95.96051008	-89.77739259	-71.47568445	-18.30170813	-70.81810624	-30.82886711
Ag (1 1 1)-1AA1,1AA2 - 19	-95.62895799	-89.4458405	-70.26046694	-19.18537356	-68.03942292	-30.33563916
Ag (1 1 1)-1AA1,1AA2 - 20	-95.39872931	-89.21561182	-70.51754513	-18.69806669	-69.09437145	-29.79093474
Ag (1 1 1)-1AA1,1AA2 - 21	-95.1180847	-88.93496721	-71.10383031	-17.8311369	-67.56259883	-31.77376325
Ag (1 1 1)-1AA1,1AA2 - 22	-94.88355227	-88.70043478	-71.13068777	-17.56974701	-67.9463772	-31.8496839
Ag (1 1 1)-1AA1,1AA2 - 23	-94.57080037	-88.38768288	-68.65753322	-19.73014965	-67.24790822	-28.6272965
Ag (1 1 1)-1AA1,1AA2 - 24	-94.32410469	-88.14098719	-69.29802649	-18.8429607	-68.42482204	-28.34558411
Ag (1 1 1)-1AA1,1AA2 - 25	-94.11731689	-87.9341994	-68.73219769	-19.2020017	-66.80368285	-28.88931946

Ag (1 1 1)-1AA1,1AA2 - 26	-93.90867175	-87.72555426	-72.93710676	-14.7884475	-66.24816672	-32.00253563
Ag (1 1 1)-1AA1,1AA2 - 27	-93.70562256	-87.52250507	-72.88353972	-14.63896535	-67.74433929	-33.01341387
Ag (1 1 1)-1AA1,1AA2 - 28	-93.37681558	-87.19369809	-74.14073624	-13.05296184	-68.11202589	-32.29343677
Ag (1 1 1)-1AA1,1AA2 - 29	-92.44908556	-86.26596806	-67.39963793	-18.86633013	-67.7451319	-27.88617753
Ag (1 1 1)-1AA1,1AA2 - 30	-91.68333781	-85.50022032	-69.58243051	-15.9177898	-65.37181647	-29.07941007
Ag (1 1 1)-1AA1,1AA2 - 31	-91.02031173	-84.83719424	-64.87196171	-19.96523252	-63.67932681	-24.66731049
Ag (1 1 1)-1AA1,1AA2 - 32	-89.40244332	-83.21932582	-68.69344715	-14.52587868	-64.48446274	-30.07005111
Ag (1 1 1)-1AA1,1AA2 - 33	-88.3464473	-82.16332981	-68.91215687	-13.25117294	-62.15608182	-28.22525963
Ag (1 1 1)-1AA1,1AA2 - 34	-88.05511372	-81.87199622	-67.2041272	-14.66786902	-61.79491134	-27.84922147
Ag (1 1 1)-1AA1,1AA2 - 35	-87.82433879	-81.6412213	-67.30645059	-14.33477071	-60.41708521	-28.67434367

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Acetic acid (AA1),Ascorbic acid (AA2).

Table C.13: Different configurations of Ag (111) surface when one formic acid (FA1), one acetic acid (AAI) and one ascorbic acid (AA2) adsorbates were adsorbed.

Structures	TE	Ads	RAE	DE	1AA2 : dEad/dNi	1AA1: dEad/dNi	1FA1: dEad/dNi
Ag (1 1 1)-1FA1,1AA1,1AA2 - 1	-150.861734	-123.8303741	-107.5034401	-16.32693393	-87.54347396	-34.52482482	-32.03930265
Ag (1 1 1)-1FA1,1AA1,1AA2 - 2	-150.0065641	-122.9752042	-106.1291328	-16.84607131	-85.95369831	-38.21117721	-28.0779689
Ag (1 1 1)-1FA1,1AA1,1AA2 - 3	-149.785321	-122.753961	-106.3561864	-16.39777461	-85.01421782	-38.32289157	-27.24176179
Ag (1 1 1)-1FA1,1AA1,1AA2 - 4	-149.4489037	-122.4175437	-111.3650833	-11.05246038	-86.34407516	-38.51226181	-31.1596755
Ag (1 1 1)-1FA1,1AA1,1AA2 - 5	-149.1671142	-122.1357542	-106.1217861	-16.01396809	-85.77100427	-30.34116226	-32.37661897
Ag (1 1 1)-1FA1,1AA1,1AA2 - 6	-148.8119601	-121.7806001	-107.5362782	-14.24432192	-86.92576997	-35.61908354	-30.48048731
Ag (1 1 1)-1FA1,1AA1,1AA2 - 7	-148.6098969	-121.5785369	-105.7566935	-15.82184336	-87.64309914	-34.61112266	-28.25160107
Ag (1 1 1)-1FA1,1AA1,1AA2 - 8	-148.203137	-121.171777	-103.2672914	-17.90448564	-82.57925781	-34.14418724	-28.31382089
Ag (1 1 1)-1FA1,1AA1,1AA2 - 9	-147.9771279	-120.9457679	-104.3921298	-16.55363808	-83.71750046	-37.72219767	-25.41549502
Ag (1 1 1)-1FA1,1AA1,1AA2 - 10	-147.7474646	-120.7161046	-105.6000817	-15.11602287	-85.32071967	-32.63672175	-29.92558202
Ag (1 1 1)-1FA1,1AA1,1AA2 - 11	-147.4859564	-120.4545965	-104.1790598	-16.27553667	-83.82176866	-30.01875427	-32.02120634
Ag (1 1 1)-1FA1,1AA1,1AA2 - 12	-147.1210526	-120.0896926	-102.7254123	-17.3642803	-85.12585938	-34.74708711	-24.90233529
Ag (1 1 1)-1FA1,1AA1,1AA2 - 13	-146.8856656	-119.8543057	-107.3435767	-12.51072898	-82.19892672	-38.24008937	-28.50159741
Ag (1 1 1)-1FA1,1AA1,1AA2 - 14	-146.685206	-119.653846	-108.6197958	-11.03405017	-76.02904538	-36.8414758	-36.59009531
Ag (1 1 1)-1FA1,1AA1,1AA2 - 15	-146.327615	-119.296255	-101.9033985	-17.39285652	-84.72931477	-31.43411365	-27.7055845
Ag (1 1 1)-1FA1,1AA1,1AA2 - 16	-145.8552494	-118.8238894	-102.3550901	-16.46879934	-81.18533305	-38.17061491	-23.81237253
Ag (1 1 1)-1FA1,1AA1,1AA2 - 17	-145.6337801	-118.6024202	-103.9886602	-14.61375998	-80.61202184	-30.72342709	-34.46028985
Ag (1 1 1)-1FA1,1AA1,1AA2 - 18	-145.4137527	-118.3823928	-105.560906	-12.82148678	-83.33306288	-32.18460915	-30.84878507
Ag (1 1 1)-1FA1,1AA1,1AA2 - 19	-145.2001743	-118.1688143	-105.8063913	-12.36242298	-82.78151042	-36.32337488	-28.55186627
Ag (1 1 1)-1FA1,1AA1,1AA2 - 20	-144.9721985	-117.9408385	-102.8296963	-15.11114225	-82.15990038	-34.24109871	-26.52340528
Ag (1 1 1)-1FA1,1AA1,1AA2 - 21	-144.7570451	-117.7256852	-101.2803123	-16.44537283	-79.07140453	-35.68985626	-28.07523404
Ag (1 1 1)-1FA1,1AA1,1AA2 - 22	-144.51243	-117.4810701	-99.70238038	-17.77868967	-83.18655493	-34.27675153	-25.44088121
Ag (1 1 1)-1FA1,1AA1,1AA2 - 23	-144.2020034	-117.1706434	-102.948038	-14.22260537	-80.45533746	-35.74630676	-30.1453253
Ag (1 1 1)-1FA1,1AA1,1AA2 - 24	-143.9040724	-116.8727125	-100.040883	-16.83182945	-82.06214282	-35.80581282	-23.03855418
Ag (1 1 1)-1FA1,1AA1,1AA2 - 25	-143.3802711	-116.3489111	-102.5598449	-13.7890662	-74.47020309	-35.23515194	-31.32148099
Ag (1 1 1)-1FA1,1AA1,1AA2 - 26	-143.127987	-116.0966271	-97.56405716	-18.53256992	-75.07101417	-35.78726492	-26.91611141

Ag (1 1 1)-1FA1,1AA1,1AA2 - 27	-142.8971107	-115.8657508	-102.4233704	-13.44238033	-79.37849811	-39.20938099	-21.83360582
Ag (1 1 1)-1FA1,1AA1,1AA2 - 28	-142.6336299	-115.6022699	-100.904821	-14.69744892	-73.18262722	-35.91568344	-31.31061394
Ag (1 1 1)-1FA1,1AA1,1AA2 - 29	-142.4334859	-115.402126	-103.4911686	-11.91095738	-80.04103694	-32.77834905	-29.07755512
Ag (1 1 1)-1FA1,1AA1,1AA2 - 30	-141.9900904	-114.9587304	-99.39388141	-15.56484898	-73.39586354	-35.68086381	-32.51359599
Ag (1 1 1)-1FA1,1AA1,1AA2 - 31	-141.7365655	-114.7052056	-101.9978401	-12.70736541	-71.16784183	-39.62243083	-35.21506151
Ag (1 1 1)-1FA1,1AA1,1AA2 - 32	-141.214763	-114.1834031	-95.68224205	-18.501161	-71.98380701	-40.29887947	-28.9815839
Ag (1 1 1)-1FA1,1AA1,1AA2 - 33	-140.998095	-113.966735	-102.7191487	-11.24758631	-80.09307014	-37.94279367	-23.46634975
Ag (1 1 1)-1FA1,1AA1,1AA2 - 34	-140.7741961	-113.7428362	-93.80298575	-19.93985041	-80.10201744	-31.01947883	-22.1844529
Ag (1 1 1)-1FA1,1AA1,1AA2 - 35	-140.5692397	-113.5378798	-98.65082379	-14.887056	-73.16821305	-33.13694111	-34.66215329
Ag (1 1 1)-1FA1,1AA1,1AA2 - 36	-140.3315873	-113.3002274	-95.30095344	-17.99927393	-77.47343284	-30.3463528	-32.8842202
Ag (1 1 1)-1FA1,1AA1,1AA2 - 37	-140.0333932	-113.0020332	-94.85387153	-18.14816168	-71.13262046	-35.10741066	-30.2928826
Ag (1 1 1)-1FA1,1AA1,1AA2 - 38	-139.6308309	-112.5994709	-94.44652129	-18.15294964	-70.17945018	-35.6764845	-31.51524956
Ag (1 1 1)-1FA1,1AA1,1AA2 - 39	-139.1901755	-112.1588155	-97.66575629	-14.49305922	-74.10898615	-36.90649474	-27.28391352
Ag (1 1 1)-1FA1,1AA1,1AA2 - 40	-138.9320314	-111.9006714	-97.48658475	-14.41408667	-69.96084922	-35.59886288	-23.70143152
Ag (1 1 1)-1FA1,1AA1,1AA2 - 41	-138.681797	-111.650437	-96.66081202	-14.98962497	-74.2531408	-35.62420104	-30.05542414
Ag (1 1 1)-1FA1,1AA1,1AA2 - 42	-138.4556229	-111.4242629	-98.24645151	-13.17781139	-74.76186609	-34.98255972	-32.107678
Ag (1 1 1)-1FA1,1AA1,1AA2 - 43	-138.2409162	-111.2095563	-95.43456435	-15.77499192	-75.51407949	-34.29594192	-29.58108983
Ag (1 1 1)-1FA1,1AA1,1AA2 - 44	-138.0098322	-110.9784723	-93.23180173	-17.74667054	-76.09541544	-36.4037478	-23.59367465
Ag (1 1 1)-1FA1,1AA1,1AA2 - 45	-137.807804	-110.776444	-97.30047166	-13.47597234	-75.80016049	-33.48099532	-31.56858852
Ag (1 1 1)-1FA1,1AA1,1AA2 - 46	-137.5566148	-110.5252548	-93.37010351	-17.15515128	-68.16499083	-34.23499985	-30.77864425
Ag (1 1 1)-1FA1,1AA1,1AA2 - 47	-137.2367793	-110.2054194	-94.56989611	-15.63552328	-69.7889631	-38.36588779	-28.58485403
Ag (1 1 1)-1FA1,1AA1,1AA2 - 48	-136.8732519	-109.8418919	-91.45389414	-18.38799779	-66.31819197	-35.20084132	-28.43437272
Ag (1 1 1)-1FA1,1AA1,1AA2 - 49	-136.6402218	-109.6088619	-95.57506177	-14.0338001	-74.49517534	-34.51430995	-27.73023427
Ag (1 1 1)-1FA1,1AA1,1AA2 - 50	-136.1704417	-109.1390817	-93.24145194	-15.89762976	-74.09280695	-32.06006011	-25.27703061
Ag (1 1 1)-1FA1,1AA1,1AA2 - 51	-135.8163591	-108.7849991	-94.32937223	-14.45562691	-72.7531352	-35.17573012	-24.49699182
Ag (1 1 1)-1FA1,1AA1,1AA2 - 52	-135.5226649	-108.491305	-90.6702745	-17.82103047	-71.71892744	-30.45535506	-25.90645873
Ag (1 1 1)-1FA1,1AA1,1AA2 - 53	-135.2491347	-108.2177747	-90.9751311	-17.24264359	-66.07393036	-35.68021498	-26.69513657
Ag (1 1 1)-1FA1,1AA1,1AA2 - 54	-135.0130711	-107.9817111	-97.45603949	-10.52567162	-70.50218989	-35.24341611	-27.75671048
Ag (1 1 1)-1FA1,1AA1,1AA2 - 55	-134.8027698	-107.7714098	-92.40427914	-15.36713069	-68.62538435	-37.0956408	-22.97588821

Ag (1 1 1)-1FA1,1AA1,1AA2 - 56	-134.5614937	-107.5301338	-91.57232245	-15.9578113	-68.87110264	-36.90259369	-27.10505532
Ag (1 1 1)-1FA1,1AA1,1AA2 - 57	-134.1001966	-107.0688366	-95.38415466	-11.68468196	-66.01937926	-37.74366276	-29.83119822
Ag (1 1 1)-1FA1,1AA1,1AA2 - 58	-133.8769536	-106.8455937	-92.87861918	-13.9669745	-67.44137917	-30.62980193	-32.75394703
Ag (1 1 1)-1FA1,1AA1,1AA2 - 59	-133.6405672	-106.6092073	-90.26841061	-16.34079666	-72.20339945	-34.08987098	-21.2546122
Ag (1 1 1)-1FA1,1AA1,1AA2 - 60	-133.349629	-106.3182691	-93.008987	-13.30928208	-66.63211787	-38.84057357	-24.28891539
Ag (1 1 1)-1FA1,1AA1,1AA2 - 61	-133.1247094	-106.0933494	-93.79593609	-12.29741333	-68.34193569	-33.28330762	-26.21349914
Ag (1 1 1)-1FA1,1AA1,1AA2 - 62	-132.2975474	-105.2661875	-89.94032994	-15.32585753	-64.05075809	-40.42146615	-22.63309532
Ag (1 1 1)-1FA1,1AA1,1AA2 - 63	-131.9390613	-104.9077013	-89.41342195	-15.49427937	-69.07735883	-31.72183279	-22.34726606
Ag (1 1 1)-1FA1,1AA1,1AA2 - 64	-131.6329517	-104.6015917	-93.20943455	-11.39215716	-68.60634075	-34.08731166	-25.76709851
Ag (1 1 1)-1FA1,1AA1,1AA2 - 65	-131.1312506	-104.0998906	-89.3046347	-14.79525589	-70.1226076	-35.19938656	-20.13318921
Ag (1 1 1)-1FA1,1AA1,1AA2 - 66	-130.7394336	-103.7080736	-96.40440253	-7.30367106	-70.64591721	-28.09312932	-25.5680081
Ag (1 1 1)-1FA1,1AA1,1AA2 - 67	-130.1468231	-103.1154631	-90.05339117	-13.06207197	-66.46815541	-33.01047051	-22.72598889
Ag (1 1 1)-1FA1,1AA1,1AA2 - 68	-128.3492727	-101.3179127	-84.8077207	-16.51019202	-60.35782904	-30.51224234	-22.45346842
Ag (1 1 1)-1FA1,1AA1,1AA2 - 69	-126.7544618	-99.72310187	-89.57205003	-10.15105184	-61.06962843	-32.34624652	-27.19108588
Ag (1 1 1)-1FA1,1AA1,1AA2 - 70	-126.5168513	-99.48549133	-82.00295124	-17.48254009	-62.59503503	-28.08837996	-22.73750972

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Formic acid (FA1) Acetic acid (AA1), Ascorbic acid (AA2).

Table C.14: Different configurations of Ag (111) surface when two formic acid (FA1), two acetic acid (AAI) and two ascorbic acid (AA2) adsorbates were adsorbed.

Structures	TE	Ads	RAE	DE	2FA1 : dEad/dNi	2AA1: dEad/dNi	2AA2: dEad/dNi
Ag (1 1 1)-2FA1,2AA1,2AA2 - 1	-279.92115	-225.858429	-193.7661237	-32.09230527	-20.57050982	-22.83212218	-93.51857818
Ag (1 1 1)-2FA1,2AA1,2AA2 - 2	-279.43988	-225.3771578	-189.713547	-35.66361078	-19.31694262	-24.72357268	-89.71772156
Ag (1 1 1)-2FA1,2AA1,2AA2 - 3	-279.19957	-225.1368498	-194.11152	-31.02532981	-20.27316497	-22.99884729	-93.53128409
Ag (1 1 1)-2FA1,2AA1,2AA2 - 4	-278.57828	-224.5155555	-191.2442477	-33.27130779	-19.83535194	-22.38971582	-92.38340891
Ag (1 1 1)-2FA1,2AA1,2AA2 - 5	-277.9206	-223.8578775	-194.4984832	-29.35939431	-21.83998387	-22.87949948	-88.06227077
Ag (1 1 1)-2FA1,2AA1,2AA2 - 6	-277.69857	-223.6358459	-189.4092744	-34.22657148	-18.41358878	-22.66277465	-92.16104741
Ag (1 1 1)-2FA1,2AA1,2AA2 - 7	-277.32776	-223.2650359	-189.5335443	-33.73149158	-18.62740392	-22.97828834	-89.85820854
Ag (1 1 1)-2FA1,2AA1,2AA2 - 8	-277.0798	-223.0170825	-193.7009866	-29.31609598	-21.30726114	-23.39758006	-85.66261061
Ag (1 1 1)-2FA1,2AA1,2AA2 - 9	-276.60687	-222.5441531	-188.3744186	-34.16973446	-18.74229448	-23.03598062	-89.16452429

Ag (1 1 1)-2FA1,2AA1,2AA2 - 10	-276.3754	-222.3126788	-189.0385141	-33.27416467	-18.06869858	-23.07339652	-88.58513571
Ag (1 1 1)-2FA1,2AA1,2AA2 - 11	-275.29035	-221.2276274	-189.973875	-31.25375242	-16.58570408	-22.4922143	-89.17068732
Ag (1 1 1)-2FA1,2AA1,2AA2 - 12	-275.00735	-220.9446302	-192.8148703	-28.12975993	-19.79742984	-22.68808103	-90.14664084
Ag (1 1 1)-2FA1,2AA1,2AA2 - 13	-274.54228	-220.47956	-186.7052201	-33.77433988	-27.19949498	-19.67008082	-92.54194352
Ag (1 1 1)-2FA1,2AA1,2AA2 - 14	-274.08704	-220.0243153	-193.7573383	-26.26697701	-20.52122854	-21.25371464	-93.88040908
Ag (1 1 1)-2FA1,2AA1,2AA2 - 15	-272.30861	-218.2458874	-185.4171324	-32.82875506	-27.78111015	-20.64927905	-94.6208995
Ag (1 1 1)-2FA1,2AA1,2AA2 - 16	-271.99392	-217.9312025	-190.0715887	-27.85961386	-23.77877801	-24.94865591	-87.13986802
Ag (1 1 1)-2FA1,2AA1,2AA2 - 17	-271.63005	-217.5673314	-189.0241632	-28.54316819	-18.27889148	-21.40524572	-93.7153899
Ag (1 1 1)-2FA1,2AA1,2AA2 - 18	-271.35868	-217.2959592	-188.0728752	-29.22308399	-25.92219695	-20.94456376	-76.30917768
Ag (1 1 1)-2FA1,2AA1,2AA2 - 19	-271.13008	-217.0673633	-189.0514669	-28.01589639	-19.9358258	-20.80983589	-96.03438168
Ag (1 1 1)-2FA1,2AA1,2AA2 - 20	-270.9004	-216.837677	-187.799397	-29.03827996	-15.92944945	-34.79077951	-95.32123727
Ag (1 1 1)-2FA1,2AA1,2AA2 - 21	-270.68447	-216.6217467	-182.2815369	-34.34020977	-28.37885732	-22.15144008	-84.9263832
Ag (1 1 1)-2FA1,2AA1,2AA2 - 22	-270.47539	-216.4126688	-182.3225877	-34.09008105	-20.90703593	-19.64703715	-89.96278193
Ag (1 1 1)-2FA1,2AA1,2AA2 - 23	-270.18765	-216.1249252	-177.3773115	-38.74761374	-10.86387667	-23.64212679	-91.71503003
Ag (1 1 1)-2FA1,2AA1,2AA2 - 24	-269.97604	-215.9133242	-178.023686	-37.88963826	-28.06611741	-19.90317629	-93.0833541
Ag (1 1 1)-2FA1,2AA1,2AA2 - 25	-269.71853	-215.6558129	-190.163012	-25.49280095	-21.17654135	-21.75556169	-91.37463231
Ag (1 1 1)-2FA1,2AA1,2AA2 - 26	-269.32383	-215.2611111	-178.6867975	-36.57431362	-15.14903337	-22.46822747	-89.84509287
Ag (1 1 1)-2FA1,2AA1,2AA2 - 27	-269.09211	-215.0293915	-188.5588814	-26.47051015	-28.65860578	-21.32325039	-87.21039463
Ag (1 1 1)-2FA1,2AA1,2AA2 - 28	-268.64902	-214.5862983	-182.992699	-31.59359935	-17.47346055	-20.88927289	-93.18213538
Ag (1 1 1)-2FA1,2AA1,2AA2 - 29	-268.33255	-214.2698283	-177.5890724	-36.68075588	-31.22115865	-21.9412526	-68.05963971
Ag (1 1 1)-2FA1,2AA1,2AA2 - 30	-268.02661	-213.9638939	-175.9276058	-38.03628804	-20.94002945	-24.50239954	-87.27807826
Ag (1 1 1)-2FA1,2AA1,2AA2 - 31	-267.75927	-213.6965549	-186.9273954	-26.76915949	-16.96168488	-21.01209778	-94.68200502
Ag (1 1 1)-2FA1,2AA1,2AA2 - 32	-267.51944	-213.4567173	-175.9146875	-37.54202975	-27.48307142	-23.99339461	-88.65581649
Ag (1 1 1)-2FA1,2AA1,2AA2 - 33	-267.18373	-213.1210108	-184.3814046	-28.7396062	-18.88744897	-21.04471022	-84.96097525
Ag (1 1 1)-2FA1,2AA1,2AA2 - 34	-266.8011	-212.7383801	-184.7518106	-27.98656948	-23.22621905	-32.09803789	-79.80714058
Ag (1 1 1)-2FA1,2AA1,2AA2 - 35	-266.59388	-212.5311647	-176.616121	-35.9150437	-21.96034392	-28.8791013	-71.02149415
Ag (1 1 1)-2FA1,2AA1,2AA2 - 36	-266.35998	-212.2972631	-178.6057638	-33.69149929	-18.65527942	-20.95288259	-96.78096063
Ag (1 1 1)-2FA1,2AA1,2AA2 - 37	-266.14179	-212.0790679	-176.918523	-35.16054499	-29.01244371	-24.21506058	-72.04735046
Ag (1 1 1)-2FA1,2AA1,2AA2 - 38	-265.77753	-211.7148134	-188.4094408	-23.30537255	-31.62138363	-22.17104213	-86.99398334

Ag (1 1 1)-2FA1,2AA1,2AA2 - 39	-265.48562	-211.4228954	-185.3051349	-26.11776049	-21.5801918	-16.49026096	-87.62728411
Ag (1 1 1)-2FA1,2AA1,2AA2 - 40	-265.23625	-211.1735311	-180.5229995	-30.65053153	-20.59429276	-39.39502093	-78.8755256
Ag (1 1 1)-2FA1,2AA1,2AA2 - 41	-264.94465	-210.8819317	-183.3996209	-27.48231083	-21.9083736	-41.19079708	-80.69911341
Ag (1 1 1)-2FA1,2AA1,2AA2 - 42	-264.62043	-210.5577148	-187.9401725	-22.61754226	-23.98394118	-24.64390782	-85.5006589
Ag (1 1 1)-2FA1,2AA1,2AA2 - 43	-264.35237	-210.2896498	-172.3419533	-37.94769649	-16.46193944	-27.2532795	-86.80456928
Ag (1 1 1)-2FA1,2AA1,2AA2 - 44	-264.14354	-210.080821	-183.1118752	-26.96894584	-11.64608641	-22.40771301	-99.21583276
Ag (1 1 1)-2FA1,2AA1,2AA2 - 45	-263.93073	-209.8680057	-171.5467785	-38.3212272	-25.5679536	-34.10501465	-63.08395795
Ag (1 1 1)-2FA1,2AA1,2AA2 - 46	-263.61905	-209.5563332	-171.6597586	-37.89657464	-26.28533153	-23.55048488	-84.64536183
Ag (1 1 1)-2FA1,2AA1,2AA2 - 47	-263.29262	-209.2299051	-180.8527973	-28.3771078	-33.43979361	-19.56420354	-74.34033643
Ag (1 1 1)-2FA1,2AA1,2AA2 - 48	-262.86527	-208.8025499	-173.2785532	-35.52399675	-17.38449195	-31.50325378	-84.99470734
Ag (1 1 1)-2FA1,2AA1,2AA2 - 49	-262.61242	-208.5496975	-176.1840534	-32.36564408	-20.27129086	-21.29703242	-86.86340796
Ag (1 1 1)-2FA1,2AA1,2AA2 - 50	-262.36876	-208.3060436	-181.175191	-27.13085265	-20.6231562	-24.86247254	-84.97969948
Ag (1 1 1)-2FA1,2AA1,2AA2 - 51	-262.05311	-207.9903881	-174.2662484	-33.72413973	-22.49538269	-17.95279189	-85.1374422
Ag (1 1 1)-2FA1,2AA1,2AA2 - 52	-261.83147	-207.7687529	-182.2424118	-25.52634104	-32.16293163	-22.80162938	-84.40300118
Ag (1 1 1)-2FA1,2AA1,2AA2 - 53	-261.40043	-207.3377146	-169.9841808	-37.3535338	-19.9975376	-31.07625476	-66.55745617
Ag (1 1 1)-2FA1,2AA1,2AA2 - 54	-261.17507	-207.1123501	-177.5764924	-29.53585772	-17.24630068	-34.46433719	-68.59175758
Ag (1 1 1)-2FA1,2AA1,2AA2 - 55	-260.97443	-206.9117091	-176.208759	-30.70295017	-20.01631201	-38.97393762	-55.68290378
Ag (1 1 1)-2FA1,2AA1,2AA2 - 56	-260.75466	-206.6919399	-172.3951994	-34.29674052	-28.86122615	-20.1724075	-59.11543173
Ag (1 1 1)-2FA1,2AA1,2AA2 - 57	-260.43538	-206.3726559	-172.5413462	-33.8313097	-30.68648899	-24.74298553	-68.49597693
Ag (1 1 1)-2FA1,2AA1,2AA2 - 58	-260.0826	-206.0198833	-175.1201847	-30.8996986	-26.55138004	-21.4252951	-65.87653413
Ag (1 1 1)-2FA1,2AA1,2AA2 - 59	-259.88228	-205.8195617	-174.2500646	-31.56949711	-20.22773955	-23.20043743	-68.39145187
Ag (1 1 1)-2FA1,2AA1,2AA2 - 60	-259.57933	-205.5166122	-174.6952901	-30.82132212	-20.21535057	-23.45244705	-69.31249182
Ag (1 1 1)-2FA1,2AA1,2AA2 - 61	-259.14376	-205.0810361	-183.8234871	-21.25754893	-17.26239222	-39.03848182	-73.60197437
Ag (1 1 1)-2FA1,2AA1,2AA2 - 62	-258.91961	-204.8568935	-172.4033399	-32.45355359	-30.63649596	-25.13257347	-68.83153378
Ag (1 1 1)-2FA1,2AA1,2AA2 - 63	-258.53796	-204.475244	-175.3321927	-29.14305127	-26.97268774	-19.95752196	-85.2342605
Ag (1 1 1)-2FA1,2AA1,2AA2 - 64	-258.26944	-204.2067218	-170.2448264	-33.96189538	-24.38178573	-31.62073795	-64.32984863
Ag (1 1 1)-2FA1,2AA1,2AA2 - 65	-258.05642	-203.9936983	-180.5901247	-23.40357358	-30.6070832	-32.56625718	-57.55140836
Ag (1 1 1)-2FA1,2AA1,2AA2 - 66	-257.76864	-203.7059188	-165.9694247	-37.73649415	-20.18332911	-17.46294329	-75.01026548
Ag (1 1 1)-2FA1,2AA1,2AA2 - 67	-257.53919	-203.4764707	-168.7212786	-34.75519218	-23.70671649	-37.32255147	-70.17288851

Ag (1 1 1)-2FA1,2AA1,2AA2 - 68	-257.32733	-203.2646131	-168.8210248	-34.44358822	-20.91721998	-37.73870791	-73.72020362
Ag (1 1 1)-2FA1,2AA1,2AA2 - 69	-257.06379	-203.0010651	-173.3591928	-29.64187229	-17.26864887	-31.83845495	-69.16493558
Ag (1 1 1)-2FA1,2AA1,2AA2 - 70	-256.73029	-202.6675664	-171.2335526	-31.43401386	-23.8841483	-33.3902077	-53.92728255
Ag (1 1 1)-2FA1,2AA1,2AA2 - 71	-256.52609	-202.463374	-179.5585302	-22.90484378	-15.56823396	-23.74143548	-84.09851841
Ag (1 1 1)-2FA1,2AA1,2AA2 - 72	-256.31151	-202.2487861	-173.8901991	-28.35858704	-20.11520052	-25.53713664	-86.7677225
Ag (1 1 1)-2FA1,2AA1,2AA2 - 73	-256.03296	-201.970244	-166.1666515	-35.80359252	-20.08867634	-36.49075116	-73.73202198
Ag (1 1 1)-2FA1,2AA1,2AA2 - 74	-255.56936	-201.5066381	-168.6558919	-32.85074615	-18.22241235	-28.13082312	-64.96156064
Ag (1 1 1)-2FA1,2AA1,2AA2 - 75	-255.36929	-201.3065664	-165.4691032	-35.83746323	-18.80215595	-29.70007462	-64.89956285
Ag (1 1 1)-2FA1,2AA1,2AA2 - 76	-254.90348	-200.8407599	-171.1167	-29.72405986	-18.89513986	-22.30242842	-81.11161484
Ag (1 1 1)-2FA1,2AA1,2AA2 - 77	-254.64037	-200.5776535	-165.9044437	-34.67320981	-14.54126923	-24.81588677	-90.36564999
Ag (1 1 1)-2FA1,2AA1,2AA2 - 78	-254.42898	-200.3662635	-174.5897716	-25.77649191	-29.1369373	-33.23416121	-60.77628225
Ag (1 1 1)-2FA1,2AA1,2AA2 - 79	-254.06888	-200.0061613	-164.6183824	-35.38777889	-21.01434499	-18.49075446	-87.17880436
Ag (1 1 1)-2FA1,2AA1,2AA2 - 80	-253.72247	-199.6597518	-176.55669	-23.10306178	-23.26538509	-18.43671803	-73.60614037
Ag (1 1 1)-2FA1,2AA1,2AA2 - 81	-253.40559	-199.3428723	-167.060347	-32.28252525	-11.21749819	-28.61232471	-82.90093733
Ag (1 1 1)-2FA1,2AA1,2AA2 - 82	-253.16793	-199.1052066	-168.5070582	-30.59814846	-20.95136508	-32.09937093	-77.04191009
Ag (1 1 1)-2FA1,2AA1,2AA2 - 83	-252.91796	-198.8552388	-179.8635103	-18.99172844	-23.06834579	-36.32213009	-72.78089447
Ag (1 1 1)-2FA1,2AA1,2AA2 - 84	-252.59622	-198.5335017	-169.5960759	-28.93742584	-19.28115132	-24.5134999	-79.04206989
Ag (1 1 1)-2FA1,2AA1,2AA2 - 85	-252.23073	-198.1680106	-168.4665563	-29.70145431	-26.23074284	-22.73777586	-69.98139884
Ag (1 1 1)-2FA1,2AA1,2AA2 - 86	-251.948	-197.8852808	-165.7700788	-32.11520201	-16.32773348	-32.99887296	-68.31371993
Ag (1 1 1)-2FA1,2AA1,2AA2 - 87	-251.59573	-197.5330145	-170.8866313	-26.64638317	-24.55940231	-17.70722105	-79.32006967
Ag (1 1 1)-2FA1,2AA1,2AA2 - 88	-251.26311	-197.2003912	-161.2289635	-35.97142774	-29.1082622	-23.46506627	-72.50717125
Ag (1 1 1)-2FA1,2AA1,2AA2 - 89	-250.93998	-196.8772562	-166.0084731	-30.86878302	-20.92676396	-28.09350573	-62.40401439
Ag (1 1 1)-2FA1,2AA1,2AA2 - 90	-250.72077	-196.6580495	-164.6194025	-32.03864706	-13.33210673	-35.77019916	-56.67636333
Ag (1 1 1)-2FA1,2AA1,2AA2 - 91	-250.41254	-196.3498153	-164.4343116	-31.91550374	-23.38110936	-17.19228141	-85.36566807
Ag (1 1 1)-2FA1,2AA1,2AA2 - 92	-250.20007	-196.1373485	-170.1203643	-26.01698421	-25.90334536	-34.23218132	-55.69671421
Ag (1 1 1)-2FA1,2AA1,2AA2 - 93	-249.95827	-195.8955535	-165.4427978	-30.45275575	-15.39060402	-16.79232321	-77.77740512
Ag (1 1 1)-2FA1,2AA1,2AA2 - 94	-249.71259	-195.6498661	-166.8424143	-28.80745182	-15.12078638	-16.8363819	-86.65519986
Ag (1 1 1)-2FA1,2AA1,2AA2 - 95	-249.18308	-195.1203649	-161.4611934	-33.6591715	-18.78550761	-23.78037103	-82.72313252
Ag (1 1 1)-2FA1,2AA1,2AA2 - 96	-248.83036	-194.7676449	-170.4672155	-24.30042938	-28.0934919	-34.64253511	-55.8006505

Ag (1 1 1)-2FA1,2AA1,2AA2 - 97	-248.57791	-194.5151934	-155.9261479	-38.58904556	-19.5748846	-24.3786493	-61.432625
Ag (1 1 1)-2FA1,2AA1,2AA2 - 98	-248.16128	-194.0985636	-158.3686035	-35.72996009	-16.86824773	-19.96482598	-70.2772944
Ag (1 1 1)-2FA1,2AA1,2AA2 - 99	-247.93719	-193.874473	-165.6512847	-28.22318835	-18.74717799	-21.90773924	-82.73161491
Ag (1 1 1)-2FA1,2AA1,2AA2 - 100	-247.57987	-193.5171514	-167.6477084	-25.869443	-13.30167104	-33.61378898	-79.25263099
Ag (1 1 1)-2FA1,2AA1,2AA2 - 101	-247.33166	-193.2689368	-165.9693912	-27.29954559	-24.54977438	-32.87005247	-50.75513837
Ag (1 1 1)-2FA1,2AA1,2AA2 - 102	-247.05577	-192.9930453	-161.6159618	-31.37708353	-21.37260194	-19.99752567	-60.91670764
Ag (1 1 1)-2FA1,2AA1,2AA2 - 103	-246.73621	-192.6734942	-171.2404325	-21.43306172	-28.17932754	-36.23888133	-62.13555552
Ag (1 1 1)-2FA1,2AA1,2AA2 - 104	-246.35641	-192.2936861	-161.3007576	-30.99292845	-20.81683591	-33.06477186	-49.74050785
Ag (1 1 1)-2FA1,2AA1,2AA2 - 105	-246.15548	-192.0927574	-166.1453433	-25.94741418	-19.10064362	-33.2239705	-54.09199096
Ag (1 1 1)-2FA1,2AA1,2AA2 - 106	-245.89103	-191.8283054	-169.7462689	-22.08203648	-21.22039025	-36.39656863	-70.89652501
Ag (1 1 1)-2FA1,2AA1,2AA2 - 107	-245.33538	-191.2726589	-152.0921393	-39.18051955	-24.82431246	-21.16038558	-54.53582996
Ag (1 1 1)-2FA1,2AA1,2AA2 - 108	-244.57757	-190.5148486	-160.8286785	-29.68617008	-27.59606766	-16.92091052	-64.45188851
Ag (1 1 1)-2FA1,2AA1,2AA2 - 109	-244.30141	-190.238694	-155.1977198	-35.04097417	-31.8368684	-20.3424789	-68.13025495
Ag (1 1 1)-2FA1,2AA1,2AA2 - 110	-243.91983	-189.8571066	-162.9320032	-26.92510342	-27.09263519	-20.73701307	-63.51479322
Ag (1 1 1)-2FA1,2AA1,2AA2 - 111	-243.65444	-189.5917152	-170.0950602	-19.49665503	-30.42034539	-21.74722734	-61.18013175
Ag (1 1 1)-2FA1,2AA1,2AA2 - 112	-243.37056	-189.3078429	-166.2732051	-23.0346378	-26.5150133	-15.67430591	-80.62642696
Ag (1 1 1)-2FA1,2AA1,2AA2 - 113	-242.93556	-188.8728401	-160.3939914	-28.47884873	-15.69885431	-36.29030015	-58.46628763
Ag (1 1 1)-2FA1,2AA1,2AA2 - 114	-241.70058	-187.6378608	-162.5684211	-25.06943971	-18.64901308	-24.99080366	-67.36365373
Ag (1 1 1)-2FA1,2AA1,2AA2 - 115	-240.99647	-186.9337526	-154.275611	-32.65814158	-15.37941891	-19.46204277	-78.09013644
Ag (1 1 1)-2FA1,2AA1,2AA2 - 116	-240.13629	-186.0735739	-155.2445618	-30.82901206	-26.56884417	-27.88031327	-58.06050125
Ag (1 1 1)-2FA1,2AA1,2AA2 - 117	-239.58684	-185.5241169	-155.9747726	-29.54934437	-16.35371802	-16.01139328	-70.08844782
Ag (1 1 1)-2FA1,2AA1,2AA2 - 118	-237.67342	-183.6107043	-147.2230179	-36.38768638	-15.21458729	-22.30507889	-79.59630307
Ag (1 1 1)-2FA1,2AA1,2AA2 - 119	-235.06017	-180.9974535	-157.4152529	-23.58220063	-28.76706243	-31.21447659	-61.55323091
Ag (1 1 1)-2FA1,2AA1,2AA2 - 120	-229.77975	-175.7170282	-151.6228456	-24.09418256	-21.68149299	-35.12655471	-56.31144059

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Formic acid (FA1) Acetic acid (AA1), Ascorbic acid (AA2).

Table C.15: Different configurations of Ag (111) surface when four formic acid (FA1), two acetic acid (AAI) and two ascorbic acid (AA2) adsorbates were adsorbed.

Structures	TE	Ads	RAE	DE	4FA1 : dEad/dNi	2AA1: dEad/dNi	2AA2: dEad/dNi
Ag (1 1 1)-4FA1,2AA1,2AA2 - 1	-347.07931	-251.3201046	-228.3144473	-23.00565733	-21.2578537	-41.37636507	-78.2828683
Ag (1 1 1)-4FA1,2AA1,2AA2 - 2	-345.90426	-250.145059	-210.13851	-40.00654902	-21.14229062	-24.56275507	-64.94446805
Ag (1 1 1)-4FA1,2AA1,2AA2 - 3	-345.61418	-249.8549717	-220.7649888	-29.08998285	-20.74209712	-22.14782801	-79.91820169
Ag (1 1 1)-4FA1,2AA1,2AA2 - 4	-344.57776	-248.818551	-220.396779	-28.42177201	-21.07881598	-42.34503928	-64.40278943
Ag (1 1 1)-4FA1,2AA1,2AA2 - 5	-343.98436	-248.2251568	-222.4103382	-25.81481853	-19.88704464	-25.20253661	-89.08329462
Ag (1 1 1)-4FA1,2AA1,2AA2 - 6	-343.64285	-247.8836402	-225.211679	-22.67196126	-23.07091181	-35.7040139	-81.1304232
Ag (1 1 1)-4FA1,2AA1,2AA2 - 7	-343.36215	-247.6029498	-225.1402344	-22.46271539	-19.28204024	-17.15773597	-99.53020733
Ag (1 1 1)-4FA1,2AA1,2AA2 - 8	-342.94182	-247.182618	-218.8421487	-28.34046937	-18.80378923	-36.43680944	-90.41294211
Ag (1 1 1)-4FA1,2AA1,2AA2 - 9	-342.48683	-246.7276217	-215.9357502	-30.79187149	-21.17950651	-22.84330408	-85.36684879
Ag (1 1 1)-4FA1,2AA1,2AA2 - 10	-341.63388	-245.8746729	-215.7953807	-30.07929221	-20.91350909	-21.94232891	-87.6069858
Ag (1 1 1)-4FA1,2AA1,2AA2 - 11	-340.98909	-245.2298814	-214.6726174	-30.55726401	-24.02518463	-31.9333872	-61.23590841
Ag (1 1 1)-4FA1,2AA1,2AA2 - 12	-340.6376	-244.8783966	-210.7997505	-34.07864616	-22.6144173	-37.48169543	-64.29976412
Ag (1 1 1)-4FA1,2AA1,2AA2 - 13	-340.38058	-244.6213775	-215.0173327	-29.60404484	-21.71363956	-19.2599046	-90.2654502
Ag (1 1 1)-4FA1,2AA1,2AA2 - 14	-340.14961	-244.3904063	-209.821892	-34.56851427	-18.48153714	-39.78566538	-72.29911471
Ag (1 1 1)-4FA1,2AA1,2AA2 - 15	-339.83051	-244.0713048	-209.8907618	-34.18054301	-18.92434147	-40.27714727	-66.45638611
Ag (1 1 1)-4FA1,2AA1,2AA2 - 16	-339.29863	-243.5394212	-218.757427	-24.78199427	-19.90039539	-36.62729248	-81.3279769
Ag (1 1 1)-4FA1,2AA1,2AA2 - 17	-339.00658	-243.2473756	-214.3446877	-28.90268795	-21.40035532	-18.13303844	-89.99263083
Ag (1 1 1)-4FA1,2AA1,2AA2 - 18	-338.63668	-242.8774754	-210.8883777	-31.98909769	-15.40708702	-37.47296483	-67.83982997
Ag (1 1 1)-4FA1,2AA1,2AA2 - 19	-338.3152	-242.555994	-214.4028471	-28.15314688	-15.80900868	-36.89871228	-69.90101557
Ag (1 1 1)-4FA1,2AA1,2AA2 - 20	-337.95511	-242.1959036	-216.2440628	-25.95184075	-18.83970069	-21.96742297	-84.33575795
Ag (1 1 1)-4FA1,2AA1,2AA2 - 21	-337.65697	-241.8977603	-220.3834494	-21.51431084	-21.95151567	-23.95332751	-86.78307599
Ag (1 1 1)-4FA1,2AA1,2AA2 - 22	-337.43106	-241.6718514	-207.6114959	-34.06035555	-20.84190989	-41.29975113	-55.53915027
Ag (1 1 1)-4FA1,2AA1,2AA2 - 23	-337.22053	-241.4613256	-216.0136366	-25.44768909	-23.16118358	-24.06533276	-80.59480802
Ag (1 1 1)-4FA1,2AA1,2AA2 - 24	-336.94534	-241.1861363	-213.3055231	-27.88061318	-18.09307586	-28.12478718	-75.09704855
Ag (1 1 1)-4FA1,2AA1,2AA2 - 25	-336.74027	-240.9810624	-208.0292127	-32.95184974	-18.57842884	-31.73616268	-66.50789367
Ag (1 1 1)-4FA1,2AA1,2AA2 - 26	-336.51558	-240.7563758	-215.6904573	-25.0659185	-15.87954176	-36.96346025	-68.77621676

Ag (1 1 1)-4FA1,2AA1,2AA2 - 27	-336.23482	-240.4756115	-207.3859492	-33.08966235	-19.17694815	-40.39705658	-62.23280739
Ag (1 1 1)-4FA1,2AA1,2AA2 - 28	-335.91307	-240.1538644	-211.0180326	-29.13583174	-19.79280976	-27.28137024	-68.81833627
Ag (1 1 1)-4FA1,2AA1,2AA2 - 29	-335.68155	-239.922342	-213.8984795	-26.02386245	-16.26895749	-35.84495951	-66.11771789
Ag (1 1 1)-4FA1,2AA1,2AA2 - 30	-335.44983	-239.6906288	-218.8486181	-20.84201073	-23.58470087	-15.63314107	-78.57681302
Ag (1 1 1)-4FA1,2AA1,2AA2 - 31	-335.04739	-239.2881828	-205.0871594	-34.20102333	-21.22928446	-31.35722067	-66.45359026
Ag (1 1 1)-4FA1,2AA1,2AA2 - 32	-334.75772	-238.9985113	-207.7467172	-31.25179414	-21.44119862	-35.28030896	-63.82179467
Ag (1 1 1)-4FA1,2AA1,2AA2 - 33	-334.45751	-238.6983031	-207.6442808	-31.05402226	-20.06417689	-28.52749968	-59.75198521
Ag (1 1 1)-4FA1,2AA1,2AA2 - 34	-334.24179	-238.4825817	-206.2225175	-32.26006416	-19.1898875	-41.06962338	-51.47800124
Ag (1 1 1)-4FA1,2AA1,2AA2 - 35	-333.98554	-238.2263378	-205.7349745	-32.49136328	-19.83639113	-37.81277285	-64.51078372
Ag (1 1 1)-4FA1,2AA1,2AA2 - 36	-333.65871	-237.8995051	-208.2944034	-29.60510166	-19.22508966	-39.21223093	-63.19537169
Ag (1 1 1)-4FA1,2AA1,2AA2 - 37	-333.44641	-237.6872094	-211.6641775	-26.02303196	-17.79472384	-32.44953572	-90.0281674
Ag (1 1 1)-4FA1,2AA1,2AA2 - 38	-333.22768	-237.4684749	-201.660037	-35.8084379	-19.13608787	-31.06064001	-74.58053051
Ag (1 1 1)-4FA1,2AA1,2AA2 - 39	-332.96823	-237.2090214	-203.8036102	-33.4054112	-19.37496774	-19.16069545	-76.87442354
Ag (1 1 1)-4FA1,2AA1,2AA2 - 40	-332.74593	-236.9867296	-203.6671072	-33.31962241	-9.91700547	-34.10653708	-79.65545163
Ag (1 1 1)-4FA1,2AA1,2AA2 - 41	-332.52351	-236.76431	-201.7356589	-35.02865116	-20.13476885	-19.32147715	-74.70337674
Ag (1 1 1)-4FA1,2AA1,2AA2 - 42	-332.3203	-236.5610945	-208.0150649	-28.54602961	-23.97854239	-21.60301852	-74.91409608
Ag (1 1 1)-4FA1,2AA1,2AA2 - 43	-332.0886	-236.3293908	-201.0592055	-35.27018521	-22.6247472	-35.41675549	-66.89778781
Ag (1 1 1)-4FA1,2AA1,2AA2 - 44	-331.88235	-236.1231415	-208.8079684	-27.31517309	-23.25459324	-35.44280847	-78.41861086
Ag (1 1 1)-4FA1,2AA1,2AA2 - 45	-331.66151	-235.9023029	-205.8634775	-30.03882543	-16.51338037	-25.24982128	-60.38241609
Ag (1 1 1)-4FA1,2AA1,2AA2 - 46	-331.43923	-235.6800279	-214.0919969	-21.58803106	-21.13577826	-39.21116251	-63.94838139
Ag (1 1 1)-4FA1,2AA1,2AA2 - 47	-331.22861	-235.4694086	-205.4890878	-29.98032079	-14.98943599	-19.49608485	-73.97677249
Ag (1 1 1)-4FA1,2AA1,2AA2 - 48	-330.82483	-235.0656234	-208.4685113	-26.59711205	-18.36062317	-20.93525137	-80.91936332
Ag (1 1 1)-4FA1,2AA1,2AA2 - 49	-330.57875	-234.8195483	-198.6559877	-36.1635606	-20.41802685	-20.16137162	-79.09714939
Ag (1 1 1)-4FA1,2AA1,2AA2 - 50	-330.32992	-234.5707167	-210.7066001	-23.86411662	-17.2548214	-18.30877371	-91.07339234
Ag (1 1 1)-4FA1,2AA1,2AA2 - 51	-330.08078	-234.3215752	-203.385612	-30.93596325	-20.86866607	-23.92864309	-81.49894056
Ag (1 1 1)-4FA1,2AA1,2AA2 - 52	-329.84174	-234.0825323	-207.8886852	-26.19384716	-17.80664736	-23.85168833	-95.71224338
Ag (1 1 1)-4FA1,2AA1,2AA2 - 53	-329.53902	-233.779814	-213.909191	-19.87062307	-17.21918088	-22.35165725	-86.17602673
Ag (1 1 1)-4FA1,2AA1,2AA2 - 54	-329.31602	-233.5568191	-206.5463359	-27.01048324	-15.72895594	-20.71196019	-76.1736487
Ag (1 1 1)-4FA1,2AA1,2AA2 - 55	-328.98758	-233.2283718	-199.3414366	-33.88693516	-18.94443125	-30.53430187	-68.05532625

Ag (1 1 1)-4FA1,2AA1,2AA2 - 56	-328.7138	-232.9546001	-208.0168909	-24.93770922	-20.29635536	-25.56290143	-67.29007878
Ag (1 1 1)-4FA1,2AA1,2AA2 - 57	-328.42116	-232.6619559	-208.0920528	-24.56990311	-20.32724669	-22.10438275	-73.8914887
Ag (1 1 1)-4FA1,2AA1,2AA2 - 58	-328.13365	-232.3744485	-209.2596843	-23.11476416	-14.67032952	-29.99016503	-80.93694857
Ag (1 1 1)-4FA1,2AA1,2AA2 - 59	-327.85054	-232.0913373	-209.6006303	-22.49070696	-19.10505176	-30.9308297	-65.76966992
Ag (1 1 1)-4FA1,2AA1,2AA2 - 60	-327.64654	-231.8873327	-197.6970504	-34.19028229	-20.70987045	-34.40598146	-78.28546005
Ag (1 1 1)-4FA1,2AA1,2AA2 - 61	-327.43624	-231.6770391	-202.6593748	-29.01766428	-22.40179432	-19.59430981	-62.57844591
Ag (1 1 1)-4FA1,2AA1,2AA2 - 62	-327.18729	-231.4280886	-204.3457842	-27.08230435	-21.61500211	-16.92723194	-79.2576286
Ag (1 1 1)-4FA1,2AA1,2AA2 - 63	-326.88609	-231.1268804	-211.793154	-19.33372636	-14.10613852	-25.70078429	-79.79082655
Ag (1 1 1)-4FA1,2AA1,2AA2 - 64	-326.57917	-230.8199619	-198.3139093	-32.50605265	-18.07050142	-30.71871948	-66.60439494
Ag (1 1 1)-4FA1,2AA1,2AA2 - 65	-326.3686	-230.6093979	-211.164533	-19.44486484	-14.67064871	-32.21050247	-74.85765184
Ag (1 1 1)-4FA1,2AA1,2AA2 - 66	-326.12842	-230.3692108	-204.9199908	-25.44922007	-13.25332061	-28.64522684	-68.2769891
Ag (1 1 1)-4FA1,2AA1,2AA2 - 67	-325.90307	-230.1438686	-211.3375873	-18.80628134	-12.56877223	-28.98520387	-91.37247881
Ag (1 1 1)-4FA1,2AA1,2AA2 - 68	-325.36806	-229.6088506	-194.315641	-35.29320957	-15.23903724	-38.91972053	-66.58274491
Ag (1 1 1)-4FA1,2AA1,2AA2 - 69	-325.1622	-229.4029957	-198.3175684	-31.0854273	-21.13490806	-21.19888013	-59.07206389
Ag (1 1 1)-4FA1,2AA1,2AA2 - 70	-324.91512	-229.1559135	-198.8228952	-30.33301833	-22.08174024	-29.28410168	-56.93979473
Ag (1 1 1)-4FA1,2AA1,2AA2 - 71	-324.66856	-228.9093553	-200.3051921	-28.60416322	-17.08294135	-38.02256527	-59.48943725
Ag (1 1 1)-4FA1,2AA1,2AA2 - 72	-324.33753	-228.5783274	-198.1855855	-30.39274186	-19.36187828	-26.24950401	-62.76459422
Ag (1 1 1)-4FA1,2AA1,2AA2 - 73	-324.09105	-228.3318451	-209.0143675	-19.31747757	-16.48520482	-20.25669498	-70.86113233
Ag (1 1 1)-4FA1,2AA1,2AA2 - 74	-323.86235	-228.10315	-200.7387758	-27.36437424	-17.84330829	-34.49197045	-51.25489345
Ag (1 1 1)-4FA1,2AA1,2AA2 - 75	-323.43877	-227.679563	-209.1693472	-18.51021588	-22.480439	-18.22874114	-74.71611854
Ag (1 1 1)-4FA1,2AA1,2AA2 - 76	-323.21233	-227.4531232	-197.3258308	-30.12729236	-14.25570251	-31.20135569	-71.21216578
Ag (1 1 1)-4FA1,2AA1,2AA2 - 77	-322.8336	-227.074398	-204.8997315	-22.17466655	-12.43050288	-26.03282631	-73.18764141
Ag (1 1 1)-4FA1,2AA1,2AA2 - 78	-322.39486	-226.6356522	-200.0974906	-26.53816161	-15.93535256	-34.5138209	-71.14514078
Ag (1 1 1)-4FA1,2AA1,2AA2 - 79	-322.04277	-226.2835663	-198.9276687	-27.35589762	-20.56163627	-33.74680084	-67.42593681
Ag (1 1 1)-4FA1,2AA1,2AA2 - 80	-321.73609	-225.9768813	-190.028539	-35.94834234	-17.82806531	-18.03049768	-87.79279293
Ag (1 1 1)-4FA1,2AA1,2AA2 - 81	-321.43625	-225.6770419	-202.8752466	-22.8017953	-13.60361155	-24.38430401	-65.17501114
Ag (1 1 1)-4FA1,2AA1,2AA2 - 82	-321.16275	-225.4035438	-189.9693081	-35.43423569	-18.58398182	-21.7279793	-60.79292146
Ag (1 1 1)-4FA1,2AA1,2AA2 - 83	-320.83098	-225.0717736	-194.5548468	-30.51692682	-14.59843967	-37.60204921	-78.64481567
Ag (1 1 1)-4FA1,2AA1,2AA2 - 84	-320.58217	-224.8229701	-198.7096652	-26.11330498	-17.66068493	-26.85347954	-65.26487809

Ag (1 1 1)-4FA1,2AA1,2AA2 - 85	-320.26039	-224.5011807	-192.9668387	-31.53434197	-21.85178482	-31.33375439	-54.74355413
Ag (1 1 1)-4FA1,2AA1,2AA2 - 86	-320.03895	-224.2797402	-193.2772219	-31.00251825	-14.68791103	-33.30624695	-79.79560592
Ag (1 1 1)-4FA1,2AA1,2AA2 - 87	-319.67645	-223.9172428	-194.6245578	-29.29268495	-23.34102287	-19.17375595	-54.62273328
Ag (1 1 1)-4FA1,2AA1,2AA2 - 88	-319.45384	-223.6946391	-201.2416489	-22.45299021	-13.99245957	-28.78847912	-78.34020558
Ag (1 1 1)-4FA1,2AA1,2AA2 - 89	-319.21957	-223.4603648	-192.3366551	-31.1237097	-20.90030846	-35.71069387	-61.16677434
Ag (1 1 1)-4FA1,2AA1,2AA2 - 90	-318.77969	-223.0204887	-198.8502796	-24.1702091	-15.49710973	-34.7076219	-63.19433184
Ag (1 1 1)-4FA1,2AA1,2AA2 - 91	-318.50486	-222.7456518	-194.6350851	-28.11056668	-19.79369199	-21.42322755	-62.08472317
Ag (1 1 1)-4FA1,2AA1,2AA2 - 92	-318.24803	-222.4888222	-189.5924292	-32.896393	-12.84323285	-17.35124497	-74.24418554
Ag (1 1 1)-4FA1,2AA1,2AA2 - 93	-317.97058	-222.2113772	-201.0268013	-21.18457587	-19.3966836	-23.86539683	-64.85450253
Ag (1 1 1)-4FA1,2AA1,2AA2 - 94	-317.63677	-221.8775607	-187.4872192	-34.39034153	-18.37901616	-31.70760747	-55.73218235
Ag (1 1 1)-4FA1,2AA1,2AA2 - 95	-317.28393	-221.5247221	-198.4342338	-23.09048826	-16.1719838	-22.80375197	-77.18254391
Ag (1 1 1)-4FA1,2AA1,2AA2 - 96	-317.03777	-221.2785616	-198.9887149	-22.28984671	-18.36188132	-19.54329787	-74.77149813
Ag (1 1 1)-4FA1,2AA1,2AA2 - 97	-316.34646	-220.5872545	-197.5440663	-23.04318826	-17.08359992	-26.83694309	-51.10089734
Ag (1 1 1)-4FA1,2AA1,2AA2 - 98	-315.90474	-220.1455314	-184.8165482	-35.32898317	-17.09706824	-22.51050371	-76.92512496
Ag (1 1 1)-4FA1,2AA1,2AA2 - 99	-315.52059	-219.7613848	-186.017752	-33.74363275	-17.10485635	-33.47416501	-71.50808475
Ag (1 1 1)-4FA1,2AA1,2AA2 - 100	-315.26978	-219.5105757	-196.7647462	-22.74582947	-13.75731533	-25.02411148	-91.20475262
Ag (1 1 1)-4FA1,2AA1,2AA2 - 101	-315.06149	-219.3022802	-185.3100209	-33.99225933	-13.74299705	-30.88886016	-71.11334573
Ag (1 1 1)-4FA1,2AA1,2AA2 - 102	-314.09802	-218.3388176	-189.605535	-28.73328259	-14.7813602	-26.12208877	-68.53855648
Ag (1 1 1)-4FA1,2AA1,2AA2 - 103	-313.49237	-217.7331676	-194.1230578	-23.61010975	-14.36125379	-16.93802116	-78.83291807
Ag (1 1 1)-4FA1,2AA1,2AA2 - 104	-313.27477	-217.5155648	-183.844187	-33.67137782	-18.07632724	-33.0045223	-64.11468545
Ag (1 1 1)-4FA1,2AA1,2AA2 - 105	-313.06712	-217.307912	-180.400678	-36.90723394	-24.28469837	-25.57931749	-46.44450007
Ag (1 1 1)-4FA1,2AA1,2AA2 - 106	-310.75173	-214.9925257	-185.7657996	-29.22672608	-18.1649188	-23.93858516	-69.20634324
Ag (1 1 1)-4FA1,2AA1,2AA2 - 107	-309.88479	-214.1255855	-185.9098272	-28.21575833	-8.73918562	-28.23859665	-77.10050612

NB: Total energy (TE), Adsorption energy (Ads), Rigid adsorption energy (RAE), Deformation energy (DE), Formic acid (FA1) Acetic acid (AA1), Ascorbic acid (AA2).

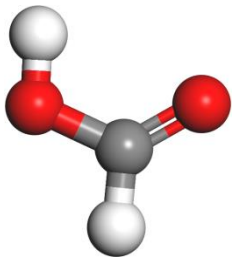
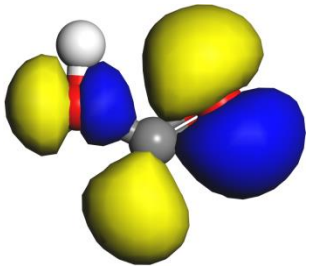
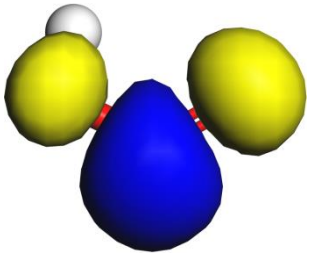
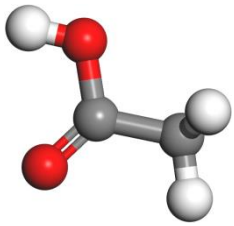
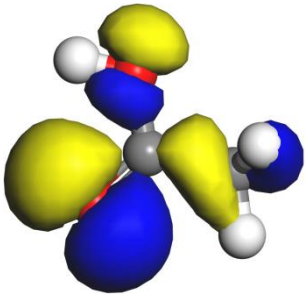
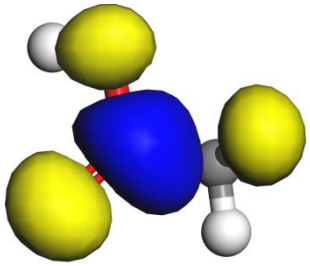
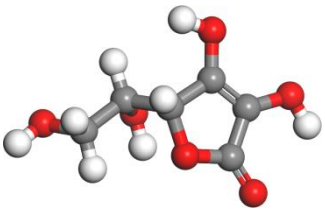
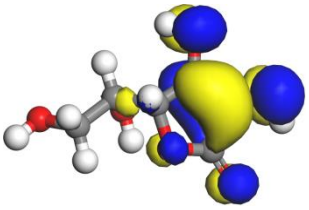
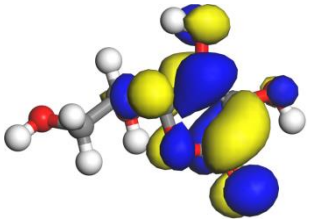
DFT-D Gas phase		
Adsorbate	**HOMO**	**LUMO**
Formic acid 		
Acetic acid 		
Ascorbic acid 		

Figure C.1: Optimized structures and the frontier molecular orbital density distributions (HOMO and LUMO).

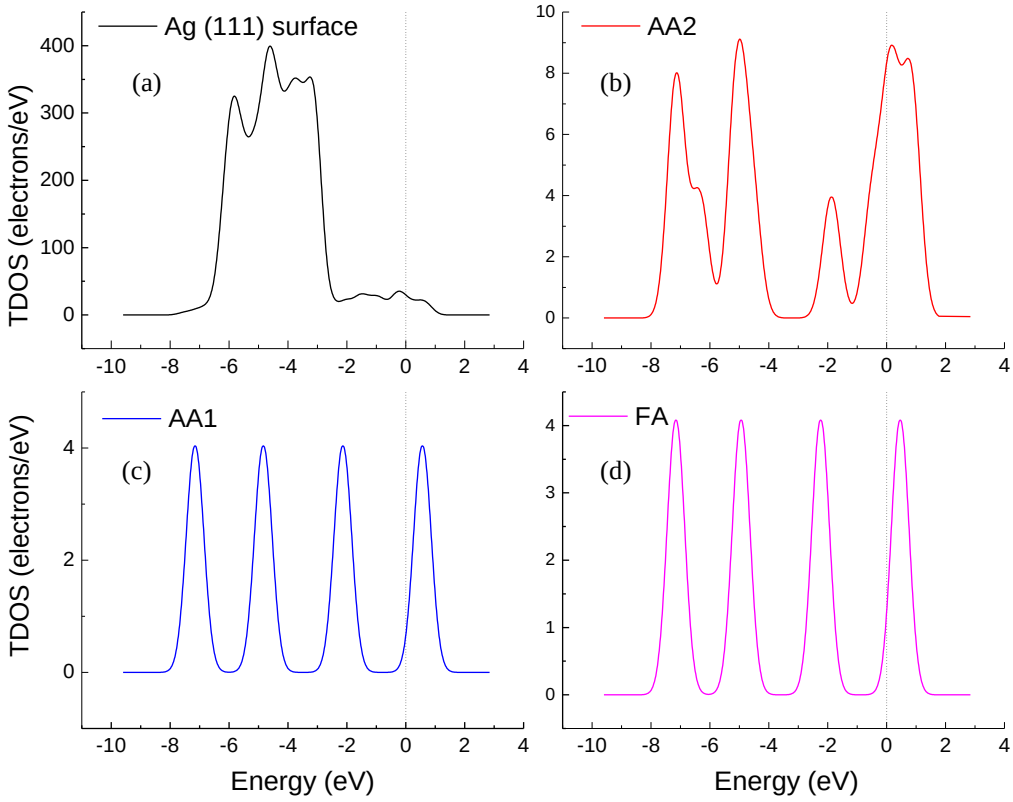


Figure C.2: Total density of states in the gas phase for (a) Ag (111) surface (b) AA2, (c) AA1 and (d) FA.

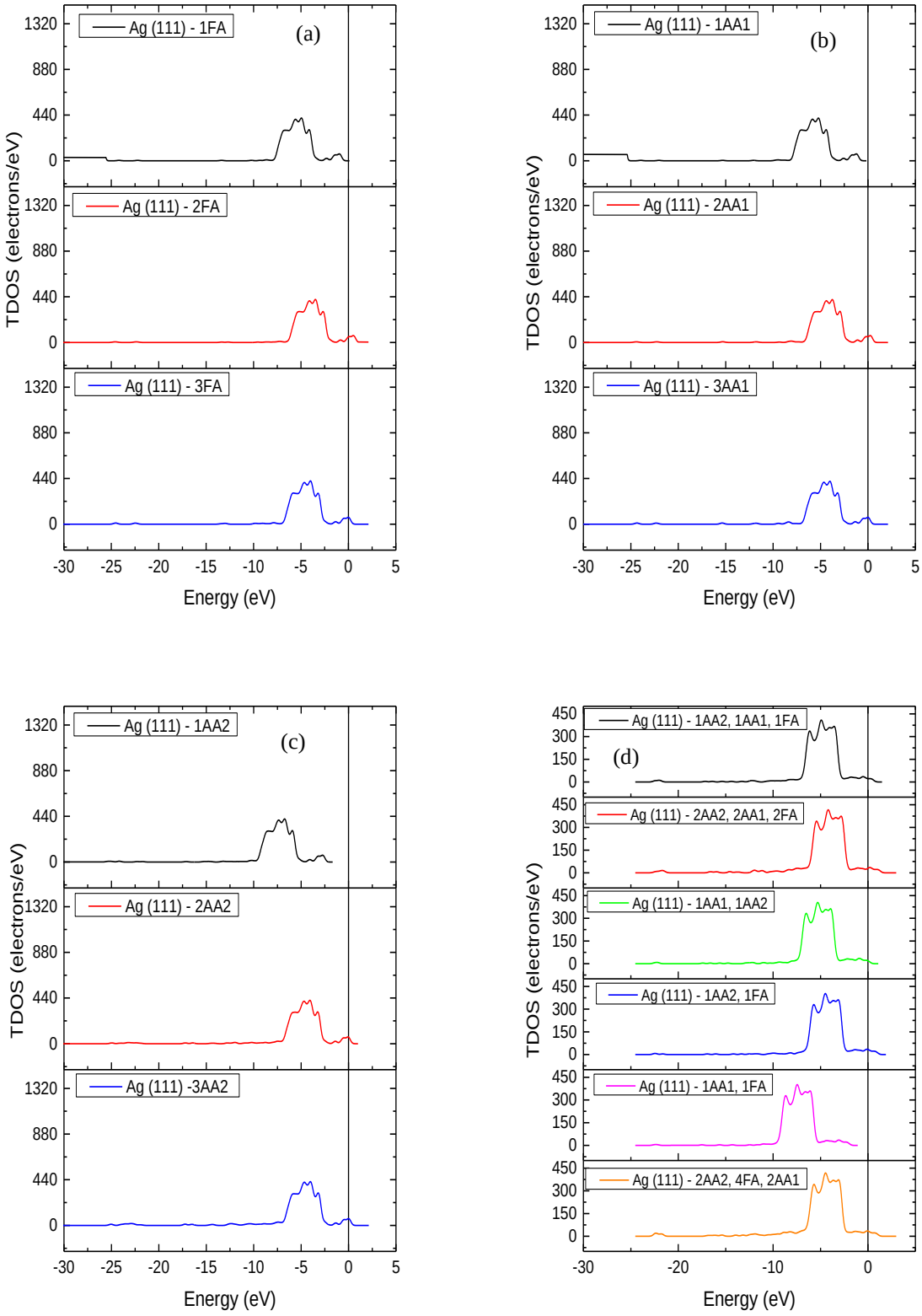


Figure C.3: The total density of states (TDOS) in the gas phase for (a) Ag (111) - 1FA, Ag (111) – 2FA and Ag (111) – 3FA (b) Ag (111) – 1AA1, Ag (111) – 2AA1 and Ag (111) – 3AA1 (c) Ag (111) – 1AA2, Ag (111) – 2AA2 and Ag (111) – 3AA2 and (d) Ag (111) surface with a mixture of NOM's. The Fermi level is indicated with a black vertical line.

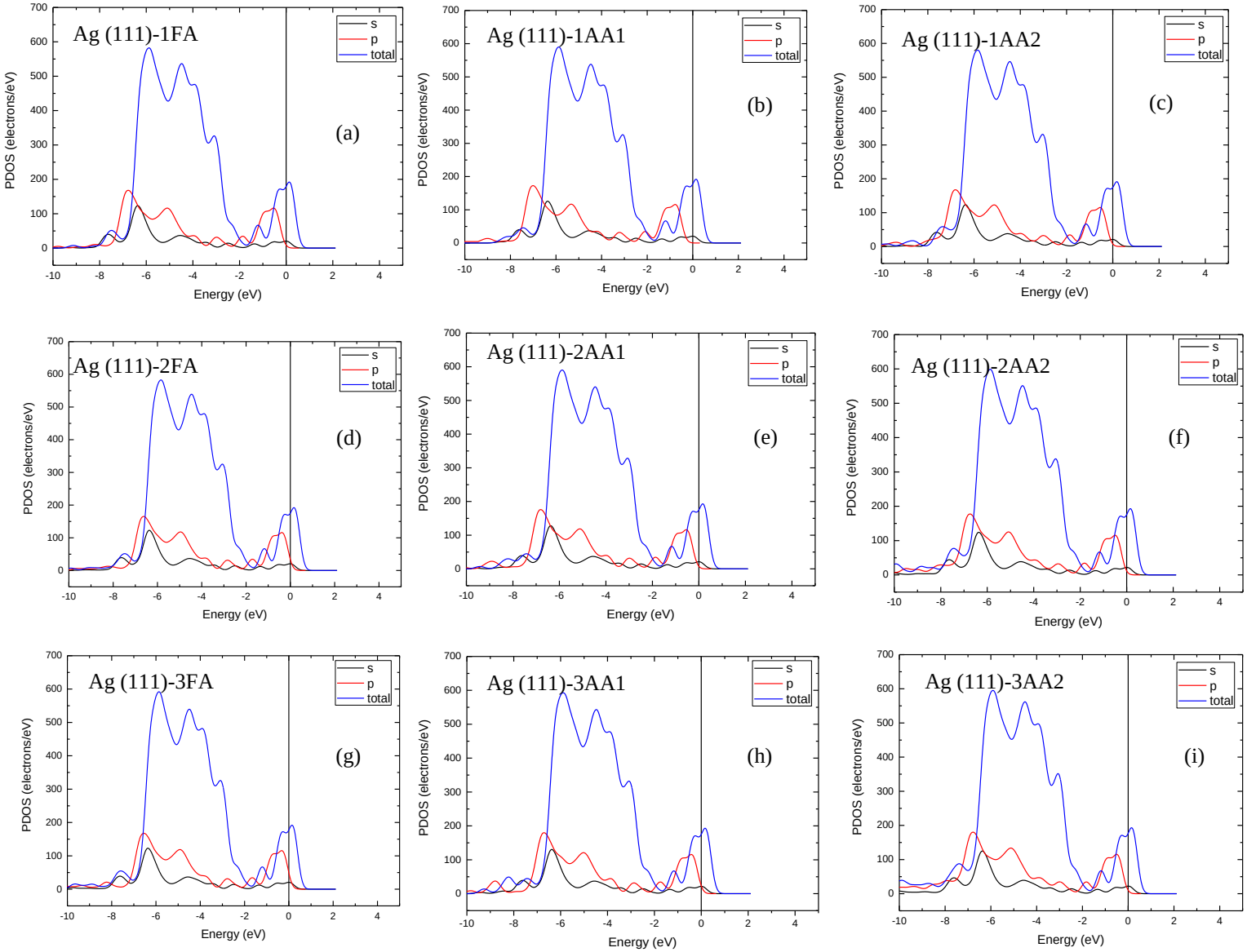


Figure C.4: Projected density of states of NOM's on Ag (111) surface (a-i) in gas phase using DFT-D/GGA level of theory.

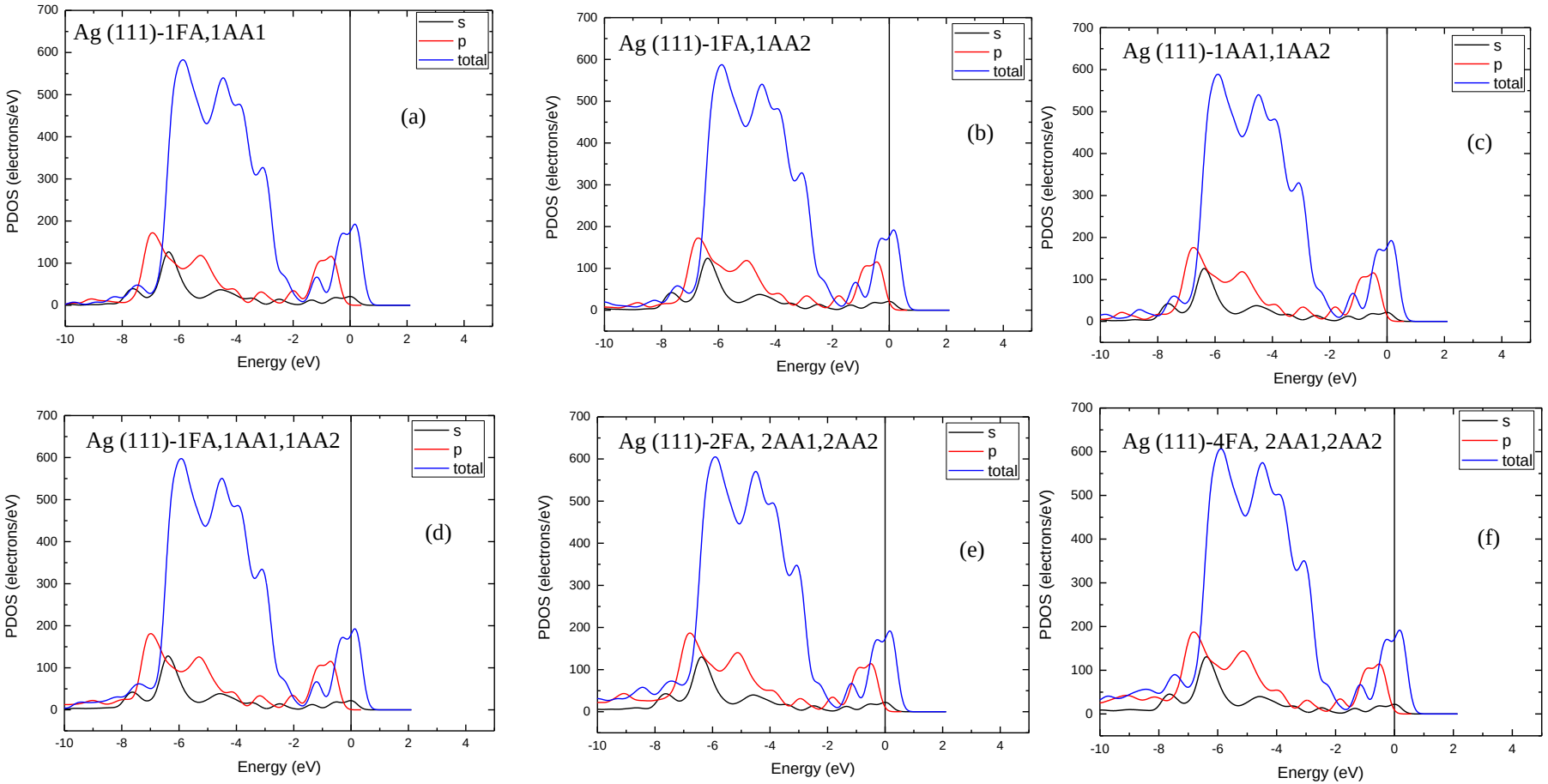


Figure C.5: Projected density of states of NOM's on Ag (111) surface (a-f) in gas phase using DFT-D/GGA level of theory.