

Supporting information for Facet dependent SERS activity of Co₃O₄

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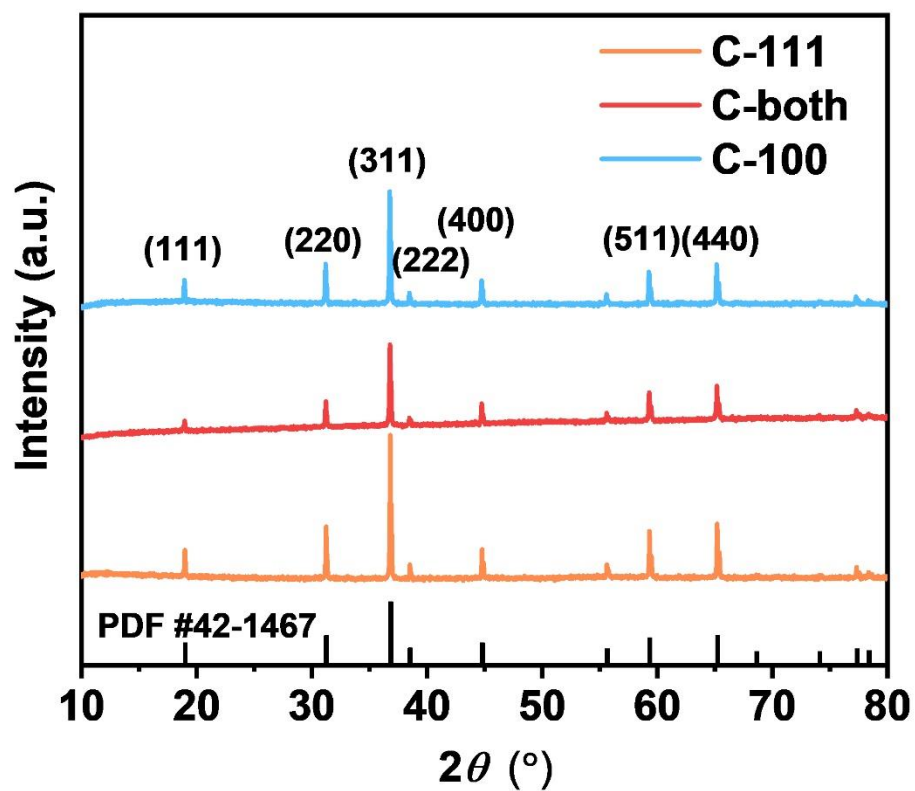


Figure S1. XRD patterns of C-100, C111 and C-both.

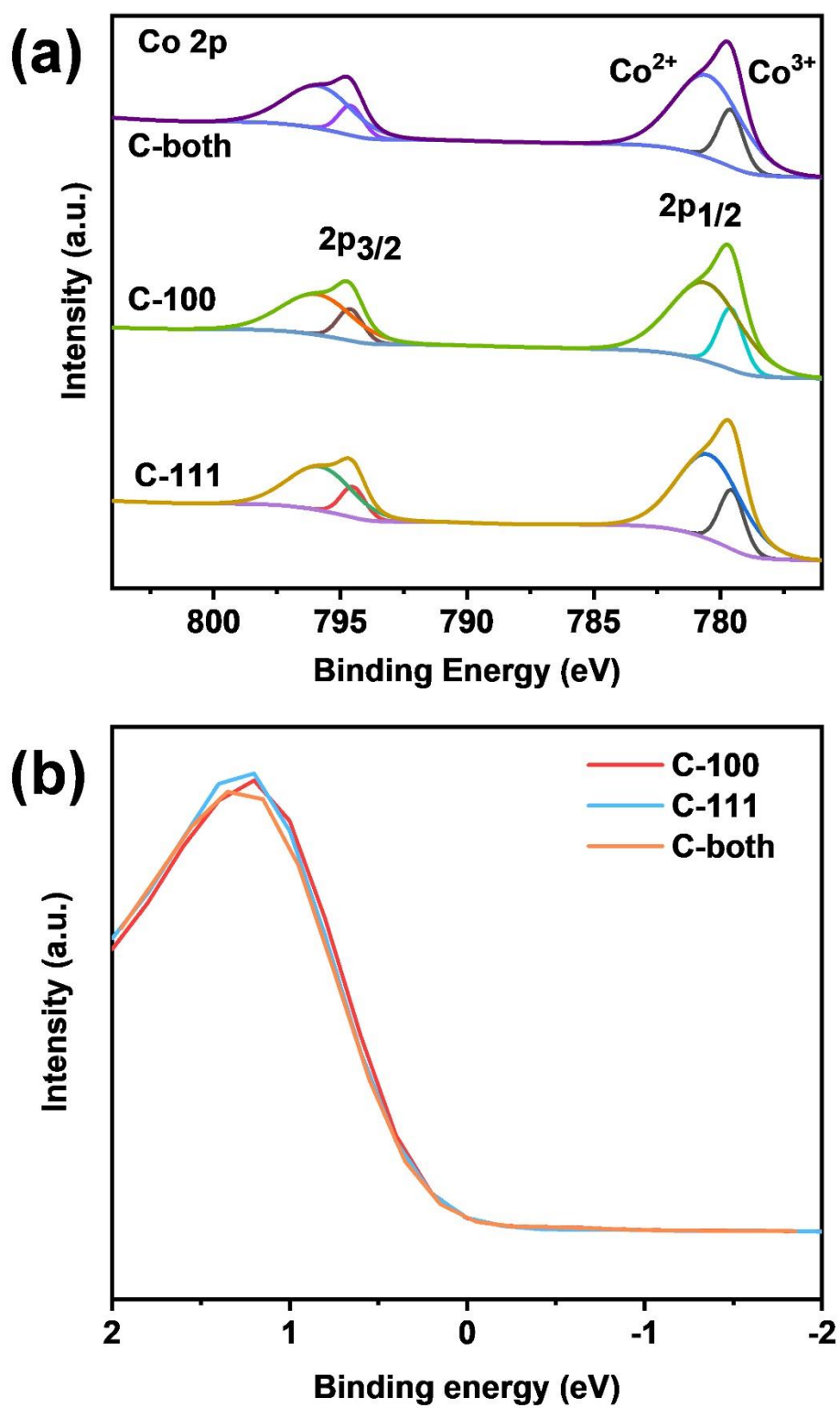


Figure S2. (a) XPS spectra of Co element. (b) VB-XPS spectra of C-100, C111 and C-both.

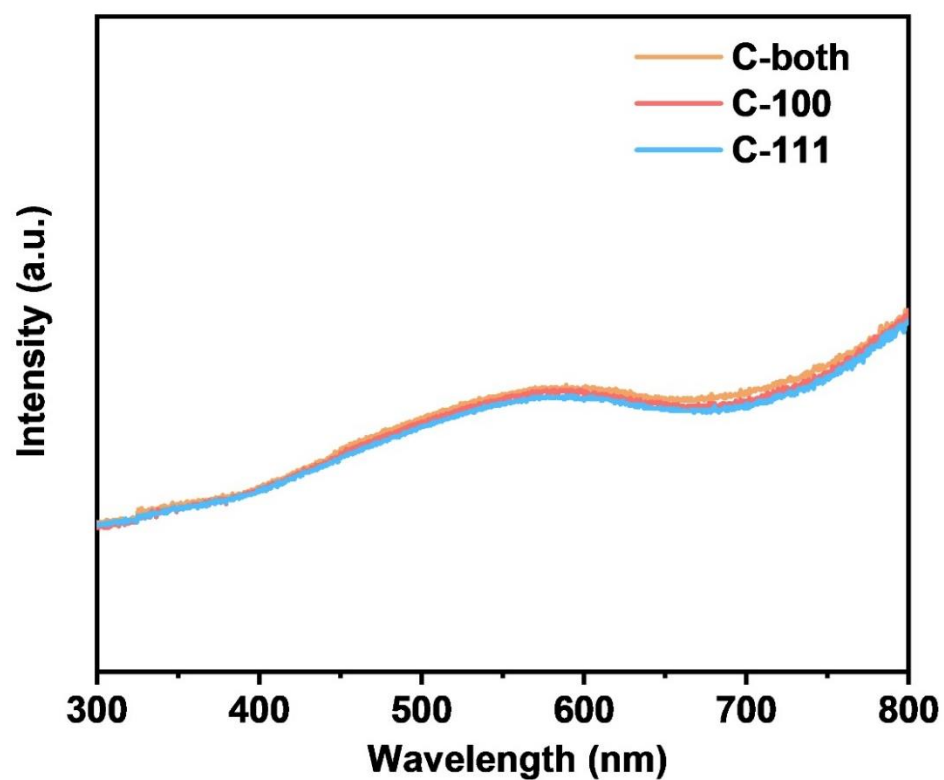


Figure S3. UV spectra of C-100, C111 and C-both.

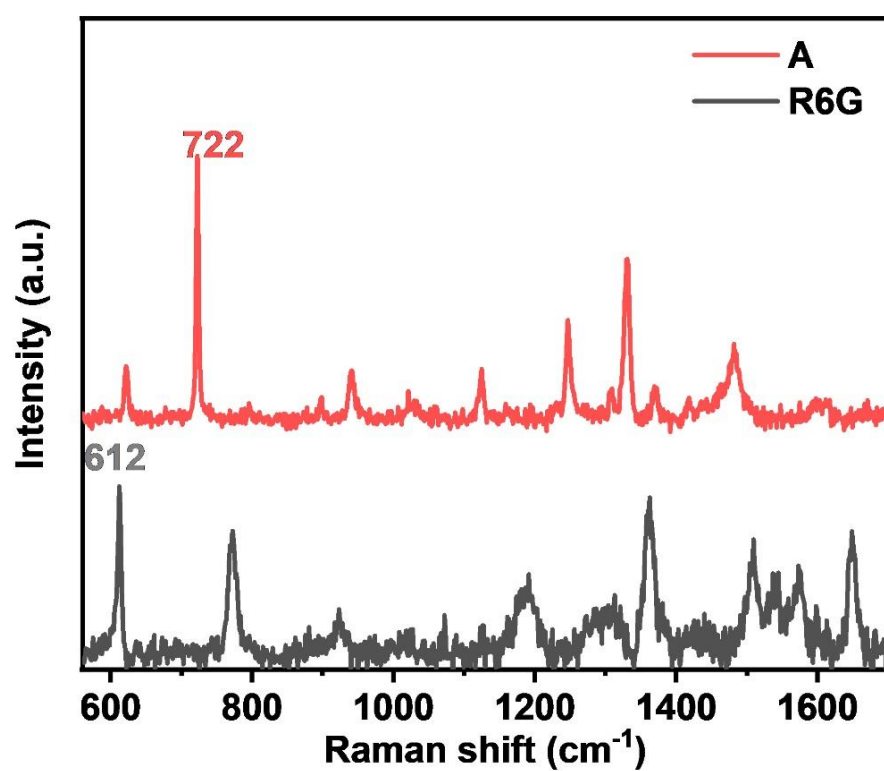


Figure S4. Raman spectra of powders A and R6G.

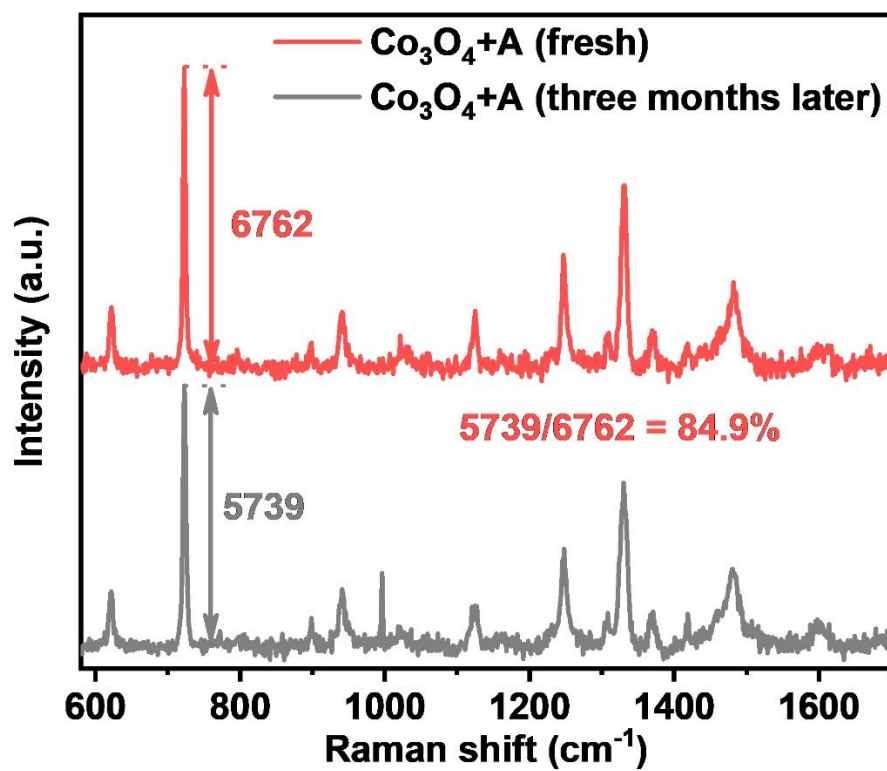


Figure S5. Fresh and three months later Raman spectrum of Co₃O₄+A.

2. Supplementary original data

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SIGMA=0.1

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EDIFFG=-0.02

NSW=2000

IALGO=38

GGA=PE

IVDW=12

IBRION=2

ISPIN=2

LMAXMIX=4

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BMIX=0.0001 !most zero,but 0 will crash some versions

AMIX_MAG=0.8

BMIX_MAG=0.0001 !most zero,but 0 will crash some versions

NPAR=8

NELM=200

LCHARG=F

LWAVE=F

LREAL=Auto

ALGO = Fast

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LDAUTYPE=2

LDAUL= 2 -1 -1 -1 -1

LDAUU= 5.9 0.0 0 0 0

LDAUJ= 0.0 0.0 0 0 0

LDAUPRINT=2

Data S1. INCAR for DFT calculation.

CONTCAR-adenine adsorbed on Co₃O₄-(100)

1.0000000000000000

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-0.0194361919000000 22.5425922527999987 0.0000000000000000

0.0000000000000000 0.0000000000000000 27.0573997497999983

Co O N C H

192 256 5 5 5

Selective dynamics

Direct

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0.6871799589999981	0.7500300410000023	0.1850800129999968	F	F	F
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0.1794157589135552	0.2499920098869235	0.2551872180455372	T	T	T
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0.3076399919999986	0.2500900129999977	0.1126000029999972	F	F	F
0.4296180059484433	0.1251984258359385	0.2558764786090132	T	T	T
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0.4422300080000028	0.2500199979999991	0.1126099949999997	F	F	F
0.3201376433272571	0.1251333177511532	0.2553345425815124	T	T	T
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0.3076500040000028	0.1251000039999965	0.1096700009999978	F	F	F
0.4297091946389691	0.2504212361775950	0.2563808490243834	T	T	T
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0.6795003913353866	0.1254142679784022	0.2554825017778586	T	T	T
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0.6792298205968935	0.2500383820652038	0.2549327360446558	T	T	T
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0.8076900780000003	0.2500900129999977	0.1125900019999975	F	F	F
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0.0576699969999979	0.5000699900000001	0.1125800000000012	F	F	F
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0.1922499860000002	0.4999800060000013	0.1126200049999966	F	F	F
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0.5576599750000000	0.5000800159999983	0.1126099949999997	F	F	F
0.6805044799264931	0.3753916652238134	0.2541969655718658	T	T	T
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0.6922500240000034	0.5000000169999979	0.1126200049999966	F	F	F
0.5699333993074017	0.3755786118698686	0.2495423456970810	T	T	T

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0.8203758039882639	0.0000570350817882	0.2551684260441097	T	T	T
0.9999700090000019	0.9303600309999993	0.0370399999999975	F	F	F
0.8750100270000019	0.8076800039999981	0.1845600059999981	F	F	F
0.8076600139999996	0.8750700339999966	0.1096799930000003	F	F	F
0.9294207402785811	0.0002156280406435	0.2551291447098771	T	T	T
0.4822059297620371	0.3200595078140589	0.3497819277322471	T	T	T
0.4336420412098400	0.4039787921461159	0.3727904107899153	T	T	T
0.5186134925452437	0.4707029591079561	0.3692834534987389	T	T	T
0.6073729933853419	0.4251737500910212	0.3367641819060673	T	T	T
0.6215702726394033	0.3222179503004787	0.3290349602563634	T	T	T
0.5238187249567376	0.3649317344949228	0.3513371417744289	T	T	T
0.4926761121413859	0.4170197089197418	0.3655138646189263	T	T	T
0.5839697638961545	0.3702586939987069	0.3412239163397125	T	T	T
0.4292146756718245	0.3471265137893236	0.3615680276615861	T	T	T
0.5738564754943155	0.4718691126075933	0.3526920099564448	T	T	T
0.4846756468461822	0.2829600264696208	0.3278526303772029	T	T	T
0.3876959414848067	0.3223774733974897	0.3612166239901079	T	T	T
0.5959211938014630	0.5149533140464362	0.3504498429289920	T	T	T
0.6649761045751683	0.3313583872589665	0.3376918557689444	T	T	T
0.6081695741145781	0.2824484985290328	0.3436065793619432	T	T	T

Data S2. CONTCAR of adenine adsorbed on C-100.

CONTCAR-adenine adsorbed on Co₃O₄-(111)

1.0000000000000000

22.5426006317000009 0.0000000000000000 0.0000000000000000

-11.2648970034999998 19.5256979472999994 0.0000000000000000

0.0000000000000000 0.0000000000000000 28.6224002838000011

Co O N C H

192 256 5 5 5

Selective dynamics

Direct

0.1668999919999976	0.0830999960000014	0.0232800010000034	F	F	F
0.0834599969999985	0.1665399930000007	0.1798300000000026	F	F	F
0.0415299969999978	0.0824600010000012	0.0799200020000015	F	F	F
0.2081000040000021	0.1659599939999978	0.2431900139999996	F	F	F
0.1675299999999993	0.2084700030000022	0.0799299979999972	F	F	F
0.0840400040000020	0.0418899989999986	0.2431900139999996	F	F	F
0.1668300030000012	0.0831499980000032	0.1420000099999967	F	F	F
0.0833696508700193	0.1665472409696183	0.2941504502794575	T	T	T
0.0414899940000026	0.2084999920000001	0.0799200020000015	F	F	F
0.2081000089999989	0.0418999999999983	0.2432200009999974	F	F	F
0.0834799969999978	0.1665299920000010	0.0030100000000033	F	F	F
0.0000899989999965	0.2498999929999997	0.1612100050000009	F	F	F
0.4168999819999968	0.0830999960000014	0.0232800010000034	F	F	F
0.3334600020000025	0.1665399930000007	0.1798300000000026	F	F	F
0.2915300020000018	0.0824600010000012	0.0799200020000015	F	F	F
0.4580999940000012	0.1659599939999978	0.2431900139999996	F	F	F
0.4175299999999993	0.2084700030000022	0.0799299979999972	F	F	F
0.3340399770000033	0.0418899989999986	0.2431900139999996	F	F	F
0.4168299930000003	0.0831499980000032	0.1420000099999967	F	F	F
0.3333303706891463	0.1664181134228004	0.2941072719431009	T	T	T
0.2914899840000018	0.2084999920000001	0.0799200020000015	F	F	F
0.4580999880000007	0.0418999999999983	0.2432200009999974	F	F	F
0.3334800080000022	0.1665299920000010	0.0030100000000033	F	F	F
0.2500899989999965	0.2498999929999997	0.1612100050000009	F	F	F
0.6668999600000021	0.0830999960000014	0.0232800010000034	F	F	F
0.5834599809999972	0.1665399930000007	0.1798300000000026	F	F	F
0.5415300020000018	0.0824600010000012	0.0799200020000015	F	F	F
0.7081000149999994	0.1659599939999978	0.2431900139999996	F	F	F
0.6675299790000011	0.2084700030000022	0.0799299979999972	F	F	F
0.5840399770000033	0.0418899989999986	0.2431900139999996	F	F	F
0.6668300139999985	0.0831499980000032	0.1420000099999967	F	F	F
0.5834018870772796	0.1664557930911784	0.2941547853226460	T	T	T
0.5414900259999982	0.2084999920000001	0.0799200020000015	F	F	F
0.7081000089999989	0.0418999999999983	0.2432200009999974	F	F	F

0.5834799860000004	0.1665299920000010	0.0030100000000033	F	F	F
0.5000899779999983	0.2498999929999997	0.1612100050000009	F	F	F
0.9168999389999968	0.0830999960000014	0.0232800010000034	F	F	F
0.8334599180000026	0.1665399930000007	0.1798300000000026	F	F	F
0.7915300230000000	0.0824600010000012	0.0799200020000015	F	F	F
0.9581000359999976	0.1659599939999978	0.2431900139999996	F	F	F
0.9175299999999993	0.2084700030000022	0.0799299979999972	F	F	F
0.8340399980000015	0.0418899989999986	0.2431900139999996	F	F	F
0.9168299930000003	0.0831499980000032	0.1420000099999967	F	F	F
0.8334177169701429	0.1665597896680379	0.2941930849081382	T	T	T
0.7914900050000000	0.2084999920000001	0.0799200020000015	F	F	F
0.9580999880000007	0.0418999999999983	0.2432200009999974	F	F	F
0.8334799650000022	0.1665299920000010	0.0030100000000033	F	F	F
0.7500899989999965	0.2498999929999997	0.1612100050000009	F	F	F
0.1668999839999969	0.3330999869999971	0.0232800010000034	F	F	F
0.0834599989999987	0.4165300259999967	0.1798300000000026	F	F	F
0.0415299909999973	0.3324599849999998	0.0799200020000015	F	F	F
0.2080999989999981	0.4159599910000011	0.2431900139999996	F	F	F
0.1675299830000014	0.4584699749999999	0.0799299979999972	F	F	F
0.0840399960000013	0.2918899809999971	0.2431900139999996	F	F	F
0.1668300010000010	0.3331500009999999	0.1420000099999967	F	F	F
0.0834694359209014	0.4166074088023297	0.2942096328025497	T	T	T
0.0414900009999997	0.4585000129999983	0.0799200020000015	F	F	F
0.2080999909999974	0.2918999939999978	0.2432200009999974	F	F	F
0.0834800100000024	0.4165300259999967	0.0030100000000033	F	F	F
0.0000899950000033	0.4999000139999978	0.1612100050000009	F	F	F
0.4168999839999969	0.3330999869999971	0.0232800010000034	F	F	F
0.3334599860000012	0.4165399899999969	0.1798300000000026	F	F	F
0.2915300009999982	0.3324599849999998	0.0799200020000015	F	F	F
0.4580999779999999	0.4159599910000011	0.2431900139999996	F	F	F
0.4175299930000023	0.4584699749999999	0.0799299979999972	F	F	F
0.3340399750000032	0.2918899809999971	0.2431900139999996	F	F	F
0.4168299800000028	0.3331500009999999	0.1420000099999967	F	F	F
0.3337672639738108	0.4175299081604700	0.2945274311080686	T	T	T
0.2914899800000015	0.4585000129999983	0.0799200020000015	F	F	F
0.4580999699999992	0.2918999939999978	0.2432200009999974	F	F	F
0.3334800100000024	0.4165300259999967	0.0030100000000033	F	F	F
0.2500899950000033	0.4999000139999978	0.1612100050000009	F	F	F
0.6668999629999988	0.3330999869999971	0.0232800010000034	F	F	F
0.5834599439999977	0.4165399899999969	0.1798300000000026	F	F	F
0.5415300009999982	0.3324599849999998	0.0799200020000015	F	F	F
0.7080999779999999	0.4159599910000011	0.2431900139999996	F	F	F
0.6675299719999970	0.4584699749999999	0.0799299979999972	F	F	F
0.5840399750000032	0.2918899809999971	0.2431900139999996	F	F	F

0.6668300219999992	0.3331500009999999	0.1420000099999967	F	F	F
0.5837432984174691	0.4163350310471298	0.2931862478669993	T	T	T
0.5414900219999979	0.4585000129999983	0.0799200020000015	F	F	F
0.7081000129999993	0.2918999939999978	0.2432200009999974	F	F	F
0.5834800100000024	0.4165300259999967	0.0030100000000033	F	F	F
0.5000899739999980	0.4999000139999978	0.1612100050000009	F	F	F
0.9168999839999969	0.3330999869999971	0.0232800010000034	F	F	F
0.8334599650000030	0.4165399899999969	0.1798300000000026	F	F	F
0.7915300220000034	0.3324599849999998	0.0799200020000015	F	F	F
0.9580999989999981	0.4159599910000011	0.2431900139999996	F	F	F
0.9175299509999988	0.4584699749999999	0.0799299979999972	F	F	F
0.8340399539999979	0.2918899809999971	0.2431900139999996	F	F	F
0.9168299589999975	0.3331500009999999	0.1420000099999967	F	F	F
0.8335275277638295	0.4166010242675982	0.2941315452161178	T	T	T
0.7914900219999979	0.4585000129999983	0.0799200020000015	F	F	F
0.9581000339999974	0.2918999939999978	0.2432200009999974	F	F	F
0.8334800310000006	0.4165300259999967	0.0030100000000033	F	F	F
0.7500899739999980	0.4999000139999978	0.1612100050000009	F	F	F
0.1668999910000011	0.5830900200000002	0.0232800010000034	F	F	F
0.0834599829999974	0.6665400110000022	0.1798300000000026	F	F	F
0.0415299940000011	0.5824599580000012	0.0799200020000015	F	F	F
0.2080999949999978	0.6659600119999993	0.2431900139999996	F	F	F
0.1675299890000019	0.7084699970000017	0.0799299979999972	F	F	F
0.0840400049999985	0.5418900270000009	0.2431900139999996	F	F	F
0.1668299849999997	0.5831499980000032	0.1420000099999967	F	F	F
0.0834335345075326	0.6665605064792232	0.2941892919096336	T	T	T
0.0414899760000011	0.7085000350000001	0.0799200020000015	F	F	F
0.2080999969999979	0.5418999910000011	0.2432200009999974	F	F	F
0.0834799820000001	0.6665299989999980	0.0030100000000033	F	F	F
0.0000899879999992	0.7498999869999992	0.1612100050000009	F	F	F
0.4168999919999976	0.5831000319999973	0.0232800010000034	F	F	F
0.3334599829999974	0.6665400110000022	0.1798300000000026	F	F	F
0.2915299940000011	0.5824599580000012	0.0799200020000015	F	F	F
0.4580999739999996	0.6659600119999993	0.2431900139999996	F	F	F
0.4175300109999966	0.7084699970000017	0.0799299979999972	F	F	F
0.3340399829999967	0.5418900270000009	0.2431900139999996	F	F	F
0.4168299640000015	0.5831499980000032	0.1420000099999967	F	F	F
0.3335676265920104	0.6664799593408446	0.2944899369371503	T	T	T
0.2914899760000011	0.7085000350000001	0.0799200020000015	F	F	F
0.4580999759999997	0.5418999910000011	0.2432200009999974	F	F	F
0.3334799820000001	0.6665299989999980	0.0030100000000033	F	F	F
0.2500900100000010	0.7498999869999992	0.1612100050000009	F	F	F
0.6668999500000012	0.5831000319999973	0.0232800010000034	F	F	F
0.5834599619999992	0.6665400110000022	0.1798300000000026	F	F	F

0.5415299940000011	0.5824599580000012	0.0799200020000015	F	F	F
0.7080999949999978	0.6659600119999993	0.2431900139999996	F	F	F
0.6675299890000019	0.7084699970000017	0.0799299979999972	F	F	F
0.5840399829999967	0.5418900270000009	0.2431900139999996	F	F	F
0.6668299849999997	0.5831499980000032	0.1420000099999967	F	F	F
0.5830532195893496	0.6663637540398570	0.2957059811045403	T	T	T
0.5414900190000012	0.7085000350000001	0.0799200020000015	F	F	F
0.7080999759999997	0.5418999910000011	0.2432200009999974	F	F	F
0.5834799610000019	0.6665299989999980	0.0030100000000033	F	F	F
0.5000899879999992	0.7498999869999992	0.1612100050000009	F	F	F
0.9168999709999994	0.5831000319999973	0.0232800010000034	F	F	F
0.8334599399999973	0.6665400110000022	0.1798300000000026	F	F	F
0.7915300160000029	0.5824599580000012	0.0799200020000015	F	F	F
0.9581000160000031	0.6659600119999993	0.2431900139999996	F	F	F
0.9175299679999966	0.7084699970000017	0.0799299979999972	F	F	F
0.8340399410000003	0.5418900270000009	0.2431900139999996	F	F	F
0.9168299640000015	0.5831499980000032	0.1420000099999967	F	F	F
0.8334939932005395	0.6667885733981977	0.2941978655895843	T	T	T
0.7914899980000030	0.7085000350000001	0.0799200020000015	F	F	F
0.9580999969999979	0.5418999910000011	0.2432200009999974	F	F	F
0.8334799820000001	0.6665299989999980	0.0030100000000033	F	F	F
0.7500900100000010	0.7498999869999992	0.1612100050000009	F	F	F
0.1668999429999971	0.8331000049999986	0.0232800010000034	F	F	F
0.0834600210000005	0.9165400329999969	0.1798300000000026	F	F	F
0.0415300120000026	0.8324599789999994	0.0799200020000015	F	F	F
0.2080999880000007	0.9159599850000006	0.2431900139999996	F	F	F
0.1675300070000034	0.9584700179999999	0.0799299979999972	F	F	F
0.0840399759999997	0.7918899989999986	0.2431900139999996	F	F	F
0.1668300030000012	0.8331500190000014	0.1420000099999967	F	F	F
0.0834108529566145	0.9165588036243041	0.2941882739036045	T	T	T
0.0414899700000007	0.9585000069999978	0.0799200020000015	F	F	F
0.2080999690000027	0.7918999629999988	0.2432200009999974	F	F	F
0.0834799539999977	0.9165299710000028	0.0030100000000033	F	F	F
0.0000899389999987	0.9998999589999968	0.1612100050000009	F	F	F
0.4168999640000024	0.8331000049999986	0.0232800010000034	F	F	F
0.3334599639999993	0.9165299710000028	0.1798300000000026	F	F	F
0.2915300120000026	0.8324599789999994	0.0799200020000015	F	F	F
0.4580999670000026	0.9159599850000006	0.2431900139999996	F	F	F
0.4175300280000016	0.9584700179999999	0.0799299979999972	F	F	F
0.3340399550000015	0.7918899989999986	0.2431900139999996	F	F	F
0.4168299809999993	0.8331500190000014	0.1420000099999967	F	F	F
0.3334197294026949	0.9165447442715708	0.2941894582342134	T	T	T
0.2914899700000007	0.9585000069999978	0.0799200020000015	F	F	F
0.4580999470000009	0.7918999629999988	0.2432200009999974	F	F	F

0.3334799750000030	0.9165299710000028	0.0030100000000033	F	F	F
0.2500899599999968	0.9998999589999968	0.1612100050000009	F	F	F
0.6668999429999971	0.8331000049999986	0.0232800010000034	F	F	F
0.5834599789999970	0.9165400329999969	0.1798300000000026	F	F	F
0.5415300120000026	0.8324599789999994	0.0799200020000015	F	F	F
0.7080999880000007	0.9159599850000006	0.2431900139999996	F	F	F
0.6675300070000034	0.9584700179999999	0.0799299979999972	F	F	F
0.5840399550000015	0.7918899989999986	0.2431900139999996	F	F	F
0.6668300030000012	0.8331500190000014	0.1420000099999967	F	F	F
0.5833632597331121	0.9165141554586630	0.2942256527894864	T	T	T
0.5414900119999970	0.9585000069999978	0.0799200020000015	F	F	F
0.7080999690000027	0.7918999629999988	0.2432200009999974	F	F	F
0.5834799539999977	0.9165299710000028	0.0030100000000033	F	F	F
0.5000899389999987	0.9998999589999968	0.1612100050000009	F	F	F
0.9168999219999989	0.8331000049999986	0.0232800010000034	F	F	F
0.8334599579999988	0.9165400329999969	0.1798300000000026	F	F	F
0.7915300330000008	0.8324599789999994	0.0799200020000015	F	F	F
0.9581000089999989	0.9159599850000006	0.2431900139999996	F	F	F
0.9175299859999981	0.9584700179999999	0.0799299979999972	F	F	F
0.8340399340000033	0.7918899989999986	0.2431900139999996	F	F	F
0.9168299809999993	0.8331500190000014	0.1420000099999967	F	F	F
0.8334221787901077	0.9165777555909050	0.2941970593119222	T	T	T
0.7914899909999988	0.9585000069999978	0.0799200020000015	F	F	F
0.9580999900000009	0.7918999629999988	0.2432200009999974	F	F	F
0.8334799750000030	0.9165299710000028	0.0030100000000033	F	F	F
0.7500899599999968	0.9998999589999968	0.1612100050000009	F	F	F
0.2114599989999988	0.0385299989999979	0.1190500060000019	F	F	F
0.1265971371650535	0.1233985871824941	0.2783836125006684	T	T	T
0.0047899990000033	0.1271499989999967	0.0387400030000009	F	F	F
0.1728399980000006	0.2113299960000035	0.2022899959999975	F	F	F
0.2115099939999965	0.1724699990000005	0.1191200009999989	F	F	F
0.1266029191949216	0.0029406523348980	0.2784155534768602	T	T	T
0.0775099949999998	0.0384799970000032	0.1191200009999989	F	F	F
0.2469443806991547	0.1233750560828641	0.2784101860454815	T	T	T
0.0001699979999970	0.2498199899999989	0.0462899999999991	F	F	F
0.1667300009999977	0.0832699959999985	0.2062699860000023	F	F	F
0.1228499999999997	0.2452100120000011	0.0387400030000009	F	F	F
0.0386699969999995	0.0771600019999994	0.2022899959999975	F	F	F
0.1229199989999969	0.1270699960000030	0.0387100040000021	F	F	F
0.0387299850000034	0.2112699930000019	0.2023200000000003	F	F	F
0.0835199970000033	0.1664700019999970	0.1144300050000027	F	F	F
0.2500902306712283	0.9999170213837245	0.2753388542363992	T	T	T
0.4614600199999970	0.0385299989999979	0.1190500060000019	F	F	F
0.3766853415084219	0.1234007363323066	0.2783851527384245	T	T	T

0.2547900140000010	0.1271499989999967	0.0387400030000009	F	F	F
0.4228399879999998	0.2113299960000035	0.2022899959999975	F	F	F
0.4615100150000018	0.1724699990000005	0.1191200009999989	F	F	F
0.3766007701931426	0.0029313788233104	0.2784100165486083	T	T	T
0.3275099949999998	0.0384799970000032	0.1191200009999989	F	F	F
0.4970041926001418	0.1233851408047526	0.2784124297832565	T	T	T
0.2501599929999969	0.2498199899999989	0.0462899999999991	F	F	F
0.4167299590000013	0.0832699959999985	0.2062699860000023	F	F	F
0.3728499999999997	0.2452100120000011	0.0387400030000009	F	F	F
0.2886700020000035	0.0771600019999994	0.2022899959999975	F	F	F
0.3729200040000009	0.1270699960000030	0.0387100040000021	F	F	F
0.2887299790000029	0.2112699930000019	0.2023200000000003	F	F	F
0.3335199819999985	0.1664700019999970	0.1144300050000027	F	F	F
0.5000904907429379	0.9999156022880057	0.2753314438847947	T	T	T
0.7114599989999988	0.0385299989999979	0.1190500060000019	F	F	F
0.6266442254965164	0.1233543847059760	0.2783962293452009	T	T	T
0.5047899719999975	0.1271499989999967	0.0387400030000009	F	F	F
0.6728400089999980	0.2113299960000035	0.2022899959999975	F	F	F
0.7115099939999965	0.1724699990000005	0.1191200009999989	F	F	F
0.6266070123307603	0.0029149710395611	0.2784069565267375	T	T	T
0.5775099949999998	0.0384799970000032	0.1191200009999989	F	F	F
0.7470255028273988	0.1233722204539682	0.2784104814143575	T	T	T
0.5001699769999988	0.2498199899999989	0.0462899999999991	F	F	F
0.6667299799999995	0.0832699959999985	0.2062699860000023	F	F	F
0.6228500209999979	0.2452100120000011	0.0387400030000009	F	F	F
0.5386699809999982	0.0771600019999994	0.2022899959999975	F	F	F
0.6229199619999974	0.1270699960000030	0.0387100040000021	F	F	F
0.5387300009999976	0.2112699930000019	0.2023200000000003	F	F	F
0.5835200240000020	0.1664700019999970	0.1144300050000027	F	F	F
0.7500899872125580	0.9999076752285357	0.2753294915405873	T	T	T
0.9614600199999970	0.0385299989999979	0.1190500060000019	F	F	F
0.8766031737756890	0.1233948958455894	0.2783866881057920	T	T	T
0.7547899509999993	0.1271499989999967	0.0387400030000009	F	F	F
0.9228399449999998	0.2113299960000035	0.2022899959999975	F	F	F
0.9615099729999983	0.1724699990000005	0.1191200009999989	F	F	F
0.8766137548732734	0.0029681384099735	0.2784139089281436	T	T	T
0.8275100170000016	0.0384799970000032	0.1191200009999989	F	F	F
0.9969896292967327	0.1233614651334572	0.2784072426776283	T	T	T
0.7501699560000006	0.2498199899999989	0.0462899999999991	F	F	F
0.9167299590000013	0.0832699959999985	0.2062699860000023	F	F	F
0.8728499999999997	0.2452100120000011	0.0387400030000009	F	F	F
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0.7887299790000029	0.2112699930000019	0.2023200000000003	F	F	F

0.8335200450000002	0.1664700019999970	0.1144300050000027	F	F	F
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0.2114599820000009	0.2885299929999974	0.1190500060000019	F	F	F
0.1266072797177020	0.3733767115145172	0.2783848348490240	T	T	T
0.0047899710000010	0.3771499839999990	0.0387400030000009	F	F	F
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0.2115099780000023	0.4224699959999967	0.1191200009999989	F	F	F
0.1266478314505112	0.2529734651981086	0.2784252414778143	T	T	T
0.0775099889999993	0.2884800029999965	0.1191200009999989	F	F	F
0.2473315222602656	0.3733387821471504	0.2782102487076101	T	T	T
0.0001699950000003	0.4998200109999971	0.0462899999999991	F	F	F
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0.1228499830000018	0.4951999970000003	0.0387400030000009	F	F	F
0.0386699829999984	0.3271599919999986	0.2022899959999975	F	F	F
0.1229199949999966	0.3770700050000002	0.0387100040000021	F	F	F
0.0387299850000034	0.4612699899999981	0.2023200000000003	F	F	F
0.0835200080000007	0.4164699990000003	0.1144300050000027	F	F	F
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0.4614600029999991	0.2885299929999974	0.1190500060000019	F	F	F
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0.4615099990000004	0.4224699959999967	0.1191200009999989	F	F	F
0.3766496197457721	0.2529773549570826	0.2785363057583991	T	T	T
0.3275099840000024	0.2884800029999965	0.1191200009999989	F	F	F
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0.3728499730000010	0.4951999970000003	0.0387400030000009	F	F	F
0.2886699829999984	0.3271599919999986	0.2022899959999975	F	F	F
0.3729199949999966	0.3770700050000002	0.0387100040000021	F	F	F
0.2887299850000034	0.4612699899999981	0.2023200000000003	F	F	F
0.3335199870000025	0.4164699990000003	0.1144300050000027	F	F	F
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0.6265820806378287	0.2528491367730319	0.2784013331193054	T	T	T
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0.5387300060000015	0.4612699899999981	0.2023200000000003	F	F	F
0.5835199870000025	0.4164699990000003	0.1144300050000027	F	F	F
0.7500906599717507	0.2499111483991477	0.2753327814582595	T	T	T
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0.9615100210000023	0.4224699959999967	0.1191200009999989	F	F	F
0.8766150622503058	0.2529444879286528	0.2784065463850055	T	T	T
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0.0386700009999998	0.5771600140000004	0.2022899959999975	F	F	F
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0.0387299779999992	0.7112699629999994	0.2023200000000003	F	F	F
0.0835199799999984	0.6664699720000016	0.1144300050000027	F	F	F
0.2500733904758759	0.4998728980619439	0.2752787551976364	T	T	T
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0.8729199750000021	0.8770700239999982	0.0387100040000021	F	F	F
0.7887299710000022	0.9612699349999971	0.2023200000000003	F	F	F
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0.6185748447569209	0.6142828423318301	0.3848561088496122	T	T	T
0.6192497377805483	0.5116334426858343	0.3840961374283062	T	T	T
0.5113849074957165	0.5130282458981806	0.3799604807952531	T	T	T
0.4794645553516670	0.5529957290149590	0.3854936672195507	T	T	T
0.5833996234777168	0.5456665016401179	0.3820535011994063	T	T	T
0.3992126349788703	0.4487398854618879	0.3813863433536794	T	T	T
0.5828932820911226	0.6479566513186362	0.3862951581461043	T	T	T
0.4615146786695763	0.4058831800303919	0.3633101315883724	T	T	T
0.3496629339547486	0.4018641539851592	0.3834280893597338	T	T	T
0.6143954033102015	0.7038900157395351	0.3885409289127596	T	T	T
0.6691761626149961	0.5391955436725951	0.3740021695842081	T	T	T
0.5949932114823048	0.4611073876582398	0.3752451725331402	T	T	T

Data S3. CONTCAR of adenine adsorbed on C-111.