

Supporting Information

The Transition Metal Surface Dependent Methane Decomposition in Graphene Chemical Vapor Deposition Growth

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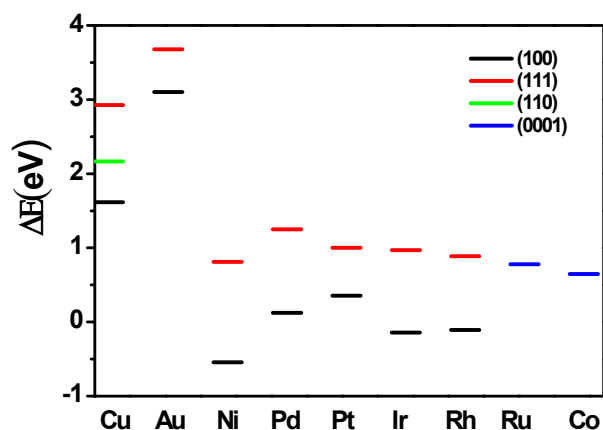
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FigureS1. Comparison of the formation energy of C atom on different catalyst surfaces.

Supplementary fractional coordinates of the first elementary step of CH₄ dissociation on Cu(111) surface

Fractional coordinate of CH₄@Cu(111)

H	C	Cu
1.0000000000000000		
8.8541743323508175	-5.1119599342346174	0.0000000000000000
0.0000000000000000	10.2239198684692383	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.2608394622802734

H	C	Cu
4	1	64

Selective dynamics

Direct

0.4232453645432296	0.3781094946187195	0.5168211909941626	T	T	T
0.2977966902672297	0.3278626358729200	0.4510452391751965	T	T	T
0.3228898812366366	0.4771764718246913	0.5025206197323576	T	T	T
0.4723747976328145	0.5032068294180981	0.4509546252401179	T	T	T
0.3790756185507326	0.4215951201456663	0.4804141356743181	T	T	T
0.0000947787396556	0.0001185186105893	0.2940038955673650	T	T	T
0.2500114367392265	-0.0000055199104440	0.2942722407858769	T	T	T
0.5002020690471455	0.0002384078523863	0.2940514783890698	T	T	T
0.7500045595708940	0.0000037721123238	0.2943013495703756	T	T	T
0.0002177957044742	0.2501851867111748	0.2944413952652796	T	T	T
0.2500479873676281	0.2501580867202101	0.2940947896908155	T	T	T
0.5002033526472760	0.2501568687582212	0.2942441090450655	T	T	T

0.7500257433939551	0.2502140550210925	0.2945258100472647	T	T	T
0.0000548341140424	0.5000970536003373	0.2953472710464682	T	T	T
0.2500757166143813	0.5001068237003593	0.2943414019993983	T	T	T
0.5002249143453783	0.5002693213251468	0.2939645356526080	T	T	T
0.7499729124630703	0.4999407715211617	0.2943950859785623	T	T	T
0.0002712643671760	0.7501379125386646	0.2944266689342288	T	T	T
0.2500767498579960	0.7501952191857163	0.2945328044457587	T	T	T
0.5002248603839555	0.7501671104504043	0.2943149620105640	T	T	T
0.7500592952952150	0.7501443995300098	0.2941192407436546	T	T	T
0.1666776939781401	0.0833092718915030	0.1962883774725680	T	T	T
0.4166989398589508	0.0833233260062547	0.1963215985201107	T	T	T
0.6665950049688639	0.0834305309222182	0.1963447528191054	T	T	T
0.9167624296508654	0.0834285055165849	0.1963559837113900	T	T	T
0.1666954616617807	0.3333467022807212	0.1960980237142586	T	T	T
0.4167869075328081	0.3334216553459935	0.1962675896640550	T	T	T
0.6666365555561227	0.3332962852853471	0.1961221505878356	T	T	T
0.9168552811372093	0.3337185902234572	0.1966876337558400	T	T	T
0.1663029047789198	0.5832198771268765	0.1967018726793628	T	T	T
0.4167295702881691	0.5833937488258447	0.1963169280417597	T	T	T
0.6666929033830628	0.5833056375727033	0.1963165846809561	T	T	T
0.9168331589314714	0.5832499085885832	0.1966428542491214	T	T	T
0.1666556834746921	0.8332662896305936	0.1961580749378196	T	T	T
0.4165597997549259	0.8333802674342692	0.1963861652776695	T	T	T
0.6666773876287465	0.8333694746097079	0.1961024150639055	T	T	T
0.9167607596223607	0.8333579304149864	0.1962933567507894	T	T	T
0.0830903649750192	0.1664595578660216	0.0978479498353773	T	T	T
0.3332512000149204	0.1666415335766335	0.0979924648200550	T	T	T
0.5831588015664283	0.1665115426517628	0.0978713638072096	T	T	T
0.8333082796144107	0.1666502226276051	0.0980916030163048	T	T	T
0.0830257161899924	0.4168869177608713	0.0979605206132541	T	T	T
0.3334771928623657	0.4168121019411188	0.0978741245090454	T	T	T
0.5831103978537172	0.4167995490233957	0.0978025285079098	T	T	T
0.8335062756341242	0.4168237025853843	0.0979932594272614	T	T	T
0.3332895200330172	0.6666396451070216	0.0981240051355180	T	T	T
0.5831134136745294	0.6665651667317999	0.0978437577280232	T	T	T
0.8333135239953415	0.6666400286674057	0.0980455987270800	T	T	T
0.3333982766071057	0.9167184569965515	0.0978920914519735	T	T	T
0.5831107928580594	0.9168433037397276	0.0978831933352924	T	T	T
0.0832053587071308	0.6665271998967700	0.0980088086201186	T	T	T
0.0831087952656134	0.9168217443509794	0.0977851217204424	T	T	T
0.8334223241859078	0.9168001649712525	0.0978306556401897	T	T	T
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F

0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F

Supplementary fractional coordinates of transition state of CH₄ dissociation on Cu(111)

H C Cu

1.0000000000000000

8.8541743323508193 -5.1119599342346200 0.0000000000000000

0.0000000000000000 10.2239198684691992 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.2608394622802983

H C Cu

4 1 64

Selective dynamics

Direct

0.6005800909773590	0.5458870107217810	0.4258486883942534	T	T	T
0.4177348462834055	0.3839981446443817	0.4097219272284827	T	T	T
0.4340082439013812	0.5651247738420312	0.4240388456113850	T	T	T
0.5684875169914675	0.6454078852595649	0.3454226610296880	T	T	T
0.4896781734800692	0.5064827230282244	0.4046140889668299	T	T	T
0.9947311931834741	0.9949721749726915	0.2945091734002037	T	T	T
0.2441350107949834	0.9947880980727808	0.2942199612720184	T	T	T
0.4947707603846817	0.9950826801152873	0.2945323944359574	T	T	T
0.7453865949711422	0.9968368988586312	0.2945130113265650	T	T	T
0.9942946925701095	0.2445811037460776	0.2943230483197499	T	T	T
0.2420875028303454	0.2430173323005584	0.2928779402103189	T	T	T

0.4954877635319506	0.2431973259875463	0.2933742218256459	T	T	T
0.7448947882036934	0.2446752677877143	0.2940502009578020	T	T	T
0.9950226807977617	0.4957178580675638	0.2943889852639656	T	T	T
0.2400276907945513	0.4942009659853548	0.2924424121447864	T	T	T
0.4918469080524832	0.4911267060998415	0.3045016169435167	T	T	T
0.7473099120404428	0.4935647588842512	0.2931290326162466	T	T	T
0.9946188282695553	0.7452130113475434	0.2942067448003123	T	T	T
0.2447892538818372	0.7453601831022751	0.2936469588605734	T	T	T
0.4965078186242137	0.7473378554296958	0.2952928892082120	T	T	T
0.7444650556755323	0.7469119156133335	0.2954487803837509	T	T	T
0.1626886934233381	0.0795981315565370	0.1959608158332202	T	T	T
0.4128660485557458	0.0797751246039182	0.1961190907203106	T	T	T
0.6630652821361311	0.0802155601081551	0.1965133600458918	T	T	T
0.9134699900611035	0.0802288151805318	0.1964456022410117	T	T	T
0.1633864781448902	0.3301998242913282	0.1954904471134515	T	T	T
0.4152334124436888	0.3342480920161547	0.1985601638703283	T	T	T
0.6628955362830110	0.3301308581879531	0.1956852638352841	T	T	T
0.9135502548515370	0.3306530263155785	0.1961784787726169	T	T	T
0.1631965522831666	0.5807122014620616	0.1958770040336165	T	T	T
0.4146200168236615	0.5797426551762538	0.1973520174966427	T	T	T
0.6613350801147568	0.5794120720273966	0.1977737028335669	T	T	T
0.9136803381012154	0.5807301357076698	0.1961531145233920	T	T	T
0.1629034424646113	0.8304428528030570	0.1957685525601417	T	T	T
0.4137730063217520	0.8299797279521971	0.1965390865773198	T	T	T
0.6628906526424029	0.8297084146564095	0.1961120331353353	T	T	T
0.9116644446354136	0.8294427780041059	0.1966549948406917	T	T	T
0.0812855646553467	0.1649898274142630	0.0977681328620719	T	T	T
0.3317060890591936	0.1662847305862699	0.0987282273441180	T	T	T
0.5814746619174718	0.1650429104769122	0.0978734917275716	T	T	T
0.8312549394793906	0.1650747231634207	0.0981657727884464	T	T	T
0.0817717252423980	0.4155997322401798	0.0977013448912010	T	T	T
0.3325365145451982	0.4157562957811483	0.0979371954793784	T	T	T
0.5812560166417851	0.4152417637187670	0.0979479670319868	T	T	T
0.8323637693550281	0.4158883229553396	0.0979283047704359	T	T	T
0.3317243070094070	0.6650532616017112	0.0982131658864938	T	T	T
0.5818301236495654	0.6652764123584020	0.0979164957216155	T	T	T
0.8305457098639663	0.6645849205970394	0.0983658388143668	T	T	T
0.3324214301640176	0.9158643548081271	0.0979338657456124	T	T	T
0.5814248192874859	0.9152745225528724	0.0979882520626355	T	T	T
0.0815973194523461	0.6652738485377638	0.0977579667904563	T	T	T
0.0812856210740875	0.9151756253338055	0.0978101165111340	T	T	T
0.8323393430565639	0.9155350989816954	0.0980415297736304	T	T	T
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F

0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F

Supplementary fractional coordinates of dissociated products of CH₃ and H on Cu(111)

H C Cu

1.0000000000000000

8.8541743323508175 -5.1119599342346174 0.0000000000000000

0.0000000000000000 10.2239198684692383 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.2608394622802734

H C Cu

4 1 64

Selective dynamics

Direct

0.4673765720727305	0.4158268387590138	0.4060633580912029	T	T	T
0.2834398216713301	0.2593496113280999	0.4017643830251350	T	T	T
0.3089295638436790	0.4447360788557570	0.4052653300384532	T	T	T
0.5927223229492382	0.6812999858638331	0.3397638568171077	T	T	T
0.3549414321018431	0.3770191884095043	0.3855010730270789	T	T	T
0.0038894143928135	0.0033627120874530	0.2935676376171145	T	T	T
0.2538072120742675	0.0015977009316733	0.2935786472702820	T	T	T
0.5036661135338207	0.0026788896724374	0.2940868510519173	T	T	T
0.7549406410757428	0.0041952402732430	0.2936785137202323	T	T	T
0.0015815860771947	0.2519830804946354	0.2932377621636016	T	T	T
0.2575083009910117	0.2570412441854017	0.3000224138598016	T	T	T

0.5064799513368764	0.2507322896031853	0.2927078974593892	T	T	T
0.7544815064153643	0.2527671803103544	0.2944324583675267	T	T	T
0.0033247300335124	0.5033980172001015	0.2941351816200227	T	T	T
0.2494526656265487	0.5031069450320154	0.2941145103930134	T	T	T
0.4999878682952161	0.4997985719057900	0.3047699478967347	T	T	T
0.7552979607472753	0.5011468954961070	0.2933087668727372	T	T	T
0.0032621607102846	0.7535470520360916	0.2940730138967855	T	T	T
0.2537078915421997	0.7535322192966857	0.2938882001809082	T	T	T
0.5041116632241768	0.7553792830070988	0.2955780922224092	T	T	T
0.7538482425474603	0.7523425540955595	0.2962313747370626	T	T	T
0.1723875641215629	0.0907137656205612	0.1980554999787119	T	T	T
0.4184850284843707	0.0853711349802521	0.1959968672959101	T	T	T
0.6685333559842099	0.0848984597787563	0.1963809424219256	T	T	T
0.9194559689063789	0.0849086714046270	0.1961810263015123	T	T	T
0.1702525811958238	0.3354925975802442	0.1965836651719277	T	T	T
0.4205055993906856	0.3383395293593020	0.1981362683772936	T	T	T
0.6696449342244145	0.3358007207232898	0.1957792169826247	T	T	T
0.9193516623370366	0.3359156589205298	0.1963659206878600	T	T	T
0.1691718085071016	0.5852201468587309	0.1964484603879680	T	T	T
0.4189761373341334	0.5846228357263508	0.1966361894500376	T	T	T
0.6652773744404192	0.5832580778042021	0.1979056829547894	T	T	T
0.9192025845604997	0.5862799426994848	0.1960602720578831	T	T	T
0.1688210376311860	0.8362472703404007	0.1955036197753410	T	T	T
0.4198878587810846	0.8346783474334190	0.1969033428769991	T	T	T
0.6694240302665716	0.8357858377367153	0.1949747560298973	T	T	T
0.9170594883686115	0.8347789905519650	0.1970303510996622	T	T	T
0.0839718994777671	0.1672291658603021	0.0980278961259884	T	T	T
0.3348707543134683	0.1685916015245891	0.0984436234740954	T	T	T
0.5841385024023712	0.1672825296469433	0.0979391690362496	T	T	T
0.8346048063838186	0.1678897881643179	0.0982798009118914	T	T	T
0.0842780884180872	0.4177201259699753	0.0979324339832695	T	T	T
0.3344987389311324	0.4174817867358419	0.0979360966915914	T	T	T
0.5844135818279688	0.4178384156611075	0.0979423770464877	T	T	T
0.8345524316502086	0.4180784346942826	0.0978776187971729	T	T	T
0.3345494682417859	0.6682845344780668	0.0979946439341916	T	T	T
0.5840991736442203	0.6671257957886159	0.0979076760103312	T	T	T
0.8341211910642606	0.6681105207598671	0.0984879883654626	T	T	T
0.3348579608343970	0.9180432532411649	0.0981086066068091	T	T	T
0.5841709619385140	0.9181836235350016	0.0975711851204484	T	T	T
0.0841047962398766	0.6673410233847943	0.0980425057168194	T	T	T
0.0845351890279151	0.9191568411221208	0.0987483870472949	T	T	T
0.8352665422488271	0.9181555550249950	0.0976048542400661	T	T	T
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F

0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F