Supporting Material for publication

Characterization of graphene/Ru(0001)

As a consequence of the existence of ripples in monolayer graphene on Ru(0001) [1, 2], the LEED pattern shows satellite spots caused by the moiré structure (Figure S1).

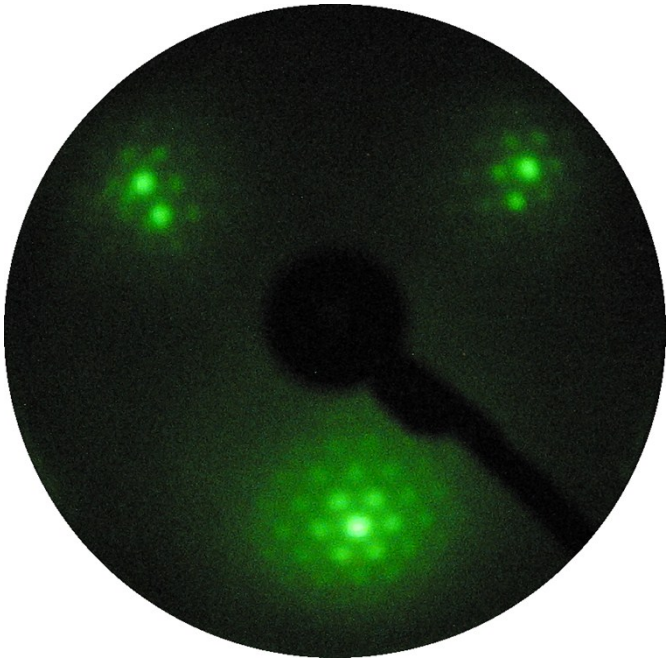

Figure S1: LEED pattern of graphene on Ru(0001), recorded at Ep = 74 eV and at room temperature.

Further characterization of the monolayer graphene has been carried out by the measurement of phonon modes (Figure S2). The presence of well-resolved ZA (out-of-plane acoustic), TA (transverse acoustic), LA (longitudinal acoustic), and LO (longitudinal optical) phonons ensures of the good order and crystalline quality of the graphene sheet.

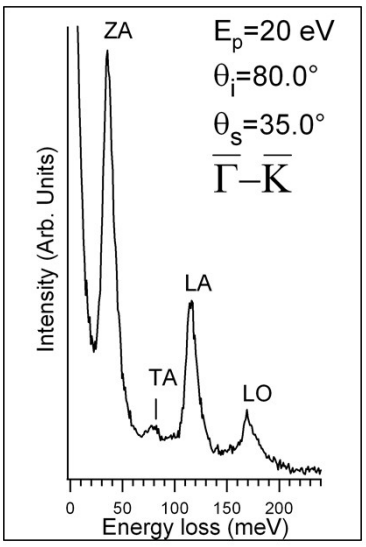

Figure S2: HREEL spectrum of the graphene/Ru(0001) for an impinging energy of 20 eV. The incidence angle is 80.0° while the scattering angle is 35.0°. The sample was oriented along the $\overline{\Gamma} - \overline{K}$ *direction.*

As concerns the microscopic investigation of air-exposed graphene/Ru(0001), the reader is referred to the previous complete study in Ref. [2] by Politano et al.

S2. Identification of the optimal etching temperature for CO stable adsorption

To complement Figure 1 in the main text, we report in Fig. S3 the intensity of the C-O stretching vibration for different etching temperatures. The maximum CO-derived signal is at 670 K.

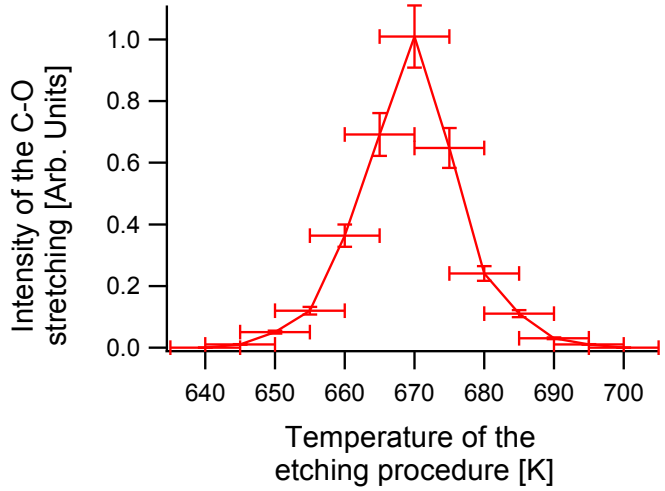

Figure S3: Intensity of the C-O stretching vibration as a function of the temperature of the etching temperature.

S3. Technical details of calculations

The energy mesh cut-off was 360 Ry in a 4×4×2 k-point mesh using the Monkhorst–Pack scheme [3]. In the optimization, the electronic ground state was found to be self-consistent using norm-conserving pseudopotentials [4] for cores; a double-ζ plus polarization basis of localized orbitals for ruthenium, carbon, and oxygen; and a double-ζ basis for hydrogen. Optimization of bond lengths and total energies were performed with an accuracy of 0.04 eV/Å and 1 meV, respectively.

S4. Testing validity of the used approaches

Firstly, we check the effect of the increase of the exactness of the calculations by decreasing the criteria of accuracy to 0.001 eV/Å and 0.1 meV. Successively, we performed the calculations for different types of van der Waals corrections. For all these checks, we study adsorption of the CO molecule on graphene with four-vacancy on Ru(0001). Results of the calculations are reported in the table:

Reference for used vdW functional	Graphene-CO distance, Å	Adsorption Energy, eV	Frequency, meV
M. Dion, H. Rydberg, E. Schroder, D. C. Langreth, and B. I. Lundqvist, Phys. Rev. Lett. 92, 246401 (2004)	2.68	-0.821	158
K. Lee, E. Murray, L. Kong, B. I. Lundqvist and D. C. Langreth, Phys. Rev. B 82, 081101 (2010)	2.69	-0.810	157
J. Klimes, D. R. Bowler, and A. Michaelides, J. Phys.: Condens. Matter 22, 022201 (2010)	2.68	-0.815	158
V. R. Cooper, Phys. Rev. B 81, 161104 (2010)	2.66	-0.828	160
K. Berland and P. Hyldgaard, Phys. Rev. B 89, 035412 (2014)	2.68	-0.825	156

O. A. Vydrov and T. Van Voorhis, J. Chem. Phys. 133, 244103 (2010)	2.70	-0.809	150
Improved accuracy	2.68	-0.8218	158

For the adsorption of CO on pristine graphene we also performed additional calculatuins by Grimme functional [S. Grimme, J. Comp. Chem. 27, 1787 (2006)] implemented in Quantum-Espresso code.Results of the calculations are shown on the next table:

Funcrional and code	Adsorption Energy, eV	Graphene-CO distance, Å
Dion-Siesta	-0.1873	2.70
Grimme-QE	-0.2504	2.66

Results of the calculations demonstrate that the choice of the functional and further increasing of the accuracy play no role. The cause of this is that the interaction between CO and graphene is dipole-dipole interaction between polar CO molecule and graphene with charge inhomogenity in vicinity of vacancy additionally doped by metallic substrate and correction that take into account London dispersion forces caused by fluctuation of charge density.

S5. Adsorption configuration

To find preferable adsorption site, we first check the adsorption energies for different sites in vicinity of the vacancy for the case of the smallest distance between graphene and metallic substrate. Results of the calculations are shown on Fig. S4. For both types of the vacancies there are several sites in vicinity with large magnitude of the adsorption energy. Further we considered only adsorption at the sites with the largest magnitude of adsorption energy.

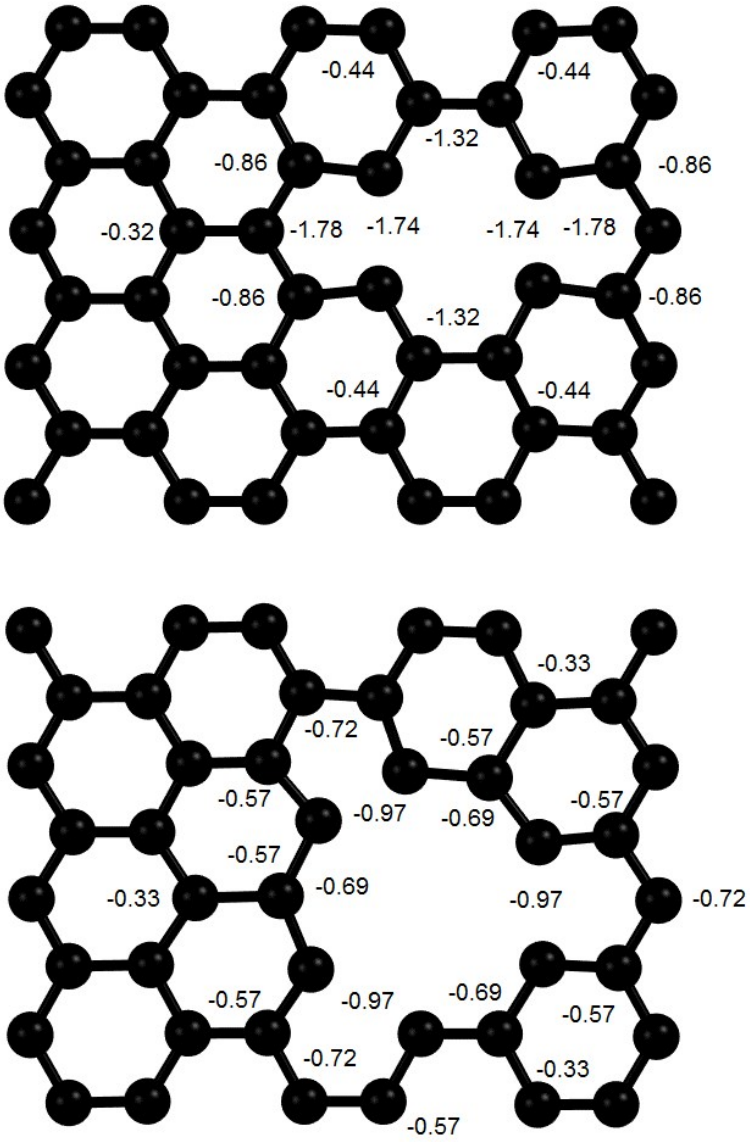

Figure S4: Adsorption energies for different sites in vicinity of bi- and four-vacancies in graphene on Ru for the shortest distance between graphene and substrate. Values are in eV.

For these selected sites, we performed two additional checks. The first is the possibility of horizontal adsorption. During the process of optimization of atomic position, CO molecules return to vertical position. The second check is adsorption on the same site with formation of C…C=O bond instead C…O=C. In the case of both vacancies the binding energy vas in order of -0.15 eV for the case of shortest distance between graphene and Ru(001). Thus, we excluded these configurations from further consideration.

References

Coordinates of optimized atomic structures.

All coordinates are scaled Cartesian. The lattice parameter is the same as in graphene 2.462 Å.

Lattice vectors of the system are:

```
 5.20000000  0.00000000  0.00000000
 0.00000000  4.00000000  0.00000000
 0.00000000  0.00000000  10.0000000
```

Adsorption on the double vacancy:

1)

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-0.60684569   0.00000453  -1.03761347  2    1  O
-0.61028181   0.00000893  -1.52972943  1    2  C
-2.28588973   0.00003111   0.01808321  1    3  C
-1.17810698   0.00003020   0.01525822  1    4  C
-0.60079472   0.00001160   0.05458895  1    5  C
 2.33229464  -0.00006612   0.04548828  1    6  C
-2.32000054   1.00342729   0.02774096  1    7  C
-1.15334428   1.00494012   0.01334650  1    8  C
-0.57869863   0.99901918   0.02189412  1    9  C
 2.30238217   0.99009910   0.03806001  1   10  C
 1.16176750   0.93682247   0.08881310  1   11  C
 0.56896634   0.94142680   0.07700554  1   12  C
-2.32006489  -1.00339749   0.02772322  1   13  C
-1.15335050  -1.00493903   0.01338016  1   14  C
-0.57869119  -0.99911796   0.02191248  1   15  C
 2.30246150  -0.99016661   0.03805396  1   16  C
 1.16174532  -0.93679144   0.08879051  1   17  C
 0.56900972  -0.94143227   0.07699418  1   18  C
-2.32677440  -1.99995763   0.03178238  1   19  C
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 1.15047468  -1.99997701   0.05599505  1   23  C
 0.57803450  -1.99997003   0.04927714  1   24  C
 2.03445472   0.47985208   0.07383862  1   25  C
 1.44612706   0.40418194   0.12899558  1   26  C
 0.27469121   0.42606377   0.06500009  1   27  C
-2.02434246   0.50009530   0.01159310  1   28  C
-1.44429405   0.50189083   0.01519406  1   29  C
-0.30711307   0.48612488   0.04992969  1   30  C
 2.00990825   1.48992201   0.04730422  1   31  C
 1.42728198   1.46580898   0.05276761  1   32  C
 0.29456885   1.47845464   0.05753376  1   33  C
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-1.45287992   1.49933341   0.02617042  1   35  C
-0.28239681   1.49355111   0.02620228  1   36  C
 2.03443834  -0.47973793   0.07385093  1   37  C
 1.44613659  -0.40421296   0.12899038  1   38  C
 0.27462757  -0.42600667   0.06487323  1   39  C
-2.02426134  -0.50009399   0.01161793  1   40  C
-1.44435967  -0.50184945   0.01524680  1   41  C
-0.30703803  -0.48604300   0.04993263  1   42  C
 2.00989157  -1.48983528   0.04730112  1   43  C
 1.42728505  -1.46579310   0.05275653  1   44  C
 0.29457860  -1.47844918   0.05754536  1   45  C
```

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2.02458412	0.49688319	1.11897937	3	61	Ru
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2)

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-1.96567806	-0.52278729	2.04131980	3	91	Ru
-0.37320951	-0.49465688	2.53592153	3	92	Ru
1.33802352	-0.48618205	1.98027246	3	93	Ru
-1.96487352	-1.48895890	1.73551010	3	94	Ru
-0.29647536	-1.49690636	2.36211731	3	95	Ru
1.33537655	-1.49755383	1.69823054	3	96	Ru
-2.33720418	-0.00029888	2.89415127	3	97	Ru
-0.69632049	0.00016712	3.48949092	3	98	Ru
1.31214581	-0.00019818	3.65484663	3	99	Ru
-2.37584562	1.03902477	2.87657055	3	100	Ru
-0.68067253	1.01031327	3.45215967	3	101	Ru
1.19652279	0.98001495	3.33752725	3	102	Ru
-2.37610240	-1.03980372	2.87691968	3	103	Ru

-0.68056938	-1.01026741	3.45329058	3	104	Ru
1.19569811	-0.97959207	3.33681547	3	105	Ru
-2.34927269	-1.99970424	2.59920673	3	106	Ru
-0.69290409	-2.00003558	3.33004874	3	107	Ru
1.18763669	-1.99980757	3.48911048	3	108	Ru
1.92776014	0.49376631	2.87670261	3	109	Ru
0.29239273	0.47009884	3.40114180	3	110	Ru
-1.41294063	0.50576543	2.93847523	3	111	Ru
1.80188168	1.49987806	2.67820403	3	112	Ru
0.26046010	1.49425298	3.27367040	3	113	Ru
-1.35857061	1.47747366	2.68514913	3	114	Ru
1.92731124	-0.49409638	2.87570574	3	115	Ru
0.29134322	-0.47149800	3.40085592	3	116	Ru
-1.41262266	-0.50586114	2.93892882	3	117	Ru
1.80155551	-1.50025643	2.67822892	3	118	Ru
0.25955011	-1.49517393	3.27215112	3	119	Ru
-1.35741814	-1.47697410	2.68517966	3	120	Ru
2.33230174	-0.00015824	3.93802272	3	121	Ru
0.64489420	-0.00015814	4.58684750	3	122	Ru
-1.25673496	-0.00004405	4.36201472	3	123	Ru
2.31564953	1.00084572	3.79751942	3	124	Ru
0.70436901	0.96945887	4.25466397	3	125	Ru
-1.20803656	1.01768756	4.37558946	3	126	Ru
2.31584712	-1.00065922	3.79765548	3	127	Ru
0.70448431	-0.96928851	4.25430564	3	128	Ru
-1.20783745	-1.01753127	4.37661258	3	129	Ru
2.24258471	-2.00013672	3.54667485	3	130	Ru
0.64503825	-1.99981713	4.36807525	3	131	Ru
-1.21515804	-1.99984022	4.22516261	3	132	Ru
-1.95514097	0.51033089	3.83086595	3	133	Ru
-0.28160545	0.49943281	4.34896593	3	134	Ru
1.62207600	0.50820314	4.52858692	3	135	Ru
-1.95245020	1.51809999	3.67322375	3	136	Ru
-0.24980686	1.50312258	4.24796228	3	137	Ru
1.62608759	1.50725222	4.31502511	3	138	Ru
-1.95511139	-0.51043805	3.83071852	3	139	Ru
-0.28173361	-0.49933181	4.34931548	3	140	Ru
1.62228754	-0.50816841	4.52843852	3	141	Ru
-1.95218378	-1.51814578	3.67330764	3	142	Ru
-0.24948187	-1.50346492	4.24852463	3	143	Ru
1.62609319	-1.50738263	4.31487763	3	144	Ru

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-0.58460680	0.00002214	-1.35282377	2	1	O
-0.61550707	0.00017990	-1.82492061	1	2	C
-2.30968855	-0.00000904	-0.28809021	1	3	C
-1.15335869	0.00006915	-0.24151905	1	4	C
-0.58053216	0.00009063	-0.27061648	1	5	C
2.32115581	-0.00002857	-0.29069381	1	6	C
-2.30396988	1.00576239	-0.29842210	1	7	C
-1.15010016	1.00710829	-0.29132789	1	8	C
-0.57757805	1.00043028	-0.32720318	1	9	C
2.32185058	0.99920382	-0.28735939	1	10	C
1.16013015	1.00003648	-0.29438133	1	11	C
0.58081340	0.98870831	-0.30582643	1	12	C
-2.30395699	-1.00566754	-0.29802820	1	13	C
-1.15027299	-1.00708312	-0.29072409	1	14	C
-0.57746958	-1.00025625	-0.32696432	1	15	C
2.32181433	-0.99931390	-0.28715354	1	16	C
1.16017566	-0.99991816	-0.29437400	1	17	C
0.58094733	-0.98877294	-0.30606928	1	18	C
-2.30754449	-1.99993609	-0.29644731	1	19	C

-1.15177226	-1.99997023	-0.32004676	1	20	C
-0.57460664	-2.00022330	-0.33540407	1	21	C
2.32600682	-1.99989949	-0.23570616	1	22	C
1.14797801	-1.99998394	-0.25845991	1	23	C
0.57060315	-2.00026403	-0.31354689	1	24	C
2.03484643	0.50398750	-0.28448429	1	25	C
1.46672072	0.52430634	-0.22133189	1	26	C
0.28983098	0.48345241	-0.27797579	1	27	C
-2.02256487	0.50005949	-0.27685254	1	28	C
-1.44590575	0.50236559	-0.25264537	1	29	C
-0.28527069	0.49583632	-0.29799026	1	30	C
2.02326789	1.49542380	-0.23767860	1	31	C
1.44506853	1.49849076	-0.26584037	1	32	C
0.28836691	1.49749810	-0.34015395	1	33	C
-2.01580049	1.50016726	-0.31188705	1	34	C
-1.44032302	1.50294134	-0.31245317	1	35	C
-0.28618583	1.50013444	-0.34820088	1	36	C
2.03464873	-0.50400507	-0.28423562	1	37	C
1.46663642	-0.52434229	-0.22102251	1	38	C
0.28983228	-0.48353330	-0.27810987	1	39	C
-2.02257007	-0.50018025	-0.27658508	1	40	C
-1.44589632	-0.50266358	-0.25221895	1	41	C
-0.28526518	-0.49631621	-0.29801252	1	42	C
2.02330580	-1.49574557	-0.23781367	1	43	C
1.44508021	-1.49859304	-0.26599114	1	44	C
0.28787351	-1.49739881	-0.34036433	1	45	C
-2.01576328	-1.50040752	-0.31157905	1	46	C
-1.44036864	-1.50307639	-0.31197073	1	47	C
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-2.07763033	0.00023292	1.11169503	3	49	Ru
-0.39733342	-0.00102395	1.20412255	3	50	Ru
1.13907354	0.00049458	0.26622626	3	51	Ru
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-0.52085129	0.99973942	1.04083559	3	53	Ru
1.05611384	0.67509464	1.11215294	3	54	Ru
-2.31643820	-0.96866319	0.97980155	3	55	Ru
-0.52056274	-1.00144562	1.03786186	3	56	Ru
1.05702888	-0.67606920	1.11087766	3	57	Ru
-2.38554973	-2.00017653	1.00647586	3	58	Ru
-0.48258843	-2.00056279	1.03733773	3	59	Ru
1.11252667	-2.00036043	0.65536755	3	60	Ru
1.98948613	0.48892928	0.94735245	3	61	Ru
0.24657805	0.51776165	0.53719266	3	62	Ru
-1.35578054	0.53801411	0.63010274	3	63	Ru
2.00951982	1.46924088	0.66357502	3	64	Ru
0.42160052	1.45226104	1.15517630	3	65	Ru
-1.43654591	1.49364362	1.00601643	3	66	Ru
1.98998555	-0.48860409	0.94702258	3	67	Ru
0.24733344	-0.51781088	0.53698970	3	68	Ru
-1.35561228	-0.53785695	0.63072069	3	69	Ru
2.01013363	-1.46890693	0.66311115	3	70	Ru
0.42186329	-1.45260732	1.15512564	3	71	Ru
-1.43714631	-1.49518668	1.00441727	3	72	Ru
2.27612329	0.00000745	1.79136441	3	73	Ru
0.47266956	-0.00040483	1.62638687	3	74	Ru
-1.19668587	0.00087980	1.74671452	3	75	Ru
2.25960679	0.98532767	1.90509987	3	76	Ru
0.54589717	0.93184826	2.24764113	3	77	Ru
-1.13760218	0.99087979	1.87616097	3	78	Ru
2.25970196	-0.98547104	1.90472511	3	79	Ru
0.54496258	-0.93040013	2.24813633	3	80	Ru
-1.13834123	-0.98961804	1.87225701	3	81	Ru

2.21147687	-2.00006432	1.85027627	3	82	Ru
0.66866381	-1.99921214	2.23489122	3	83	Ru
-1.11109325	-1.99974218	1.89244801	3	84	Ru
-2.05357088	0.50090624	2.03022802	3	85	Ru
-0.37064519	0.49362896	2.33157335	3	86	Ru
1.37010265	0.47410898	2.11919276	3	87	Ru
-2.03478719	1.49655179	1.86747417	3	88	Ru
-0.22311722	1.49058505	1.94139841	3	89	Ru
1.36554563	1.47820007	1.65966462	3	90	Ru
-2.05347230	-0.50081667	2.02987809	3	91	Ru
-0.37225998	-0.49352723	2.33212602	3	92	Ru
1.37004604	-0.47448054	2.11758762	3	93	Ru
-2.03447631	-1.49660592	1.86720612	3	94	Ru
-0.22364868	-1.48899063	1.94057431	3	95	Ru
1.36582376	-1.47846125	1.65926629	3	96	Ru
-2.25904523	0.00016243	2.94046892	3	97	Ru
-0.68187390	0.00010241	3.39578901	3	98	Ru
1.23721055	-0.00010261	3.53230244	3	99	Ru
-2.32337193	1.02149288	2.90073597	3	100	Ru
-0.66508723	1.00034275	3.38198081	3	101	Ru
1.16173692	0.95968408	3.14095048	3	102	Ru
-2.32322430	-1.02112270	2.90054433	3	103	Ru
-0.66596725	-1.00044115	3.38217204	3	104	Ru
1.16197205	-0.95878167	3.13984692	3	105	Ru
-2.31916459	-1.99982256	2.76102036	3	106	Ru
-0.64969059	-1.99993452	3.29466424	3	107	Ru
1.15071678	-1.99965708	3.28968490	3	108	Ru
2.02238900	0.48901091	2.88562212	3	109	Ru
0.26651741	0.46639438	3.16585034	3	110	Ru
-1.36018240	0.50039967	2.80923412	3	111	Ru
1.89797565	1.50478752	2.70854360	3	112	Ru
0.21992147	1.49481638	3.05512275	3	113	Ru
-1.37089167	1.49741441	2.78624150	3	114	Ru
2.02265051	-0.48768717	2.88359350	3	115	Ru
0.26523869	-0.46724759	3.16721878	3	116	Ru
-1.36036491	-0.50026885	2.80893877	3	117	Ru
1.89824192	-1.50437008	2.70878312	3	118	Ru
0.22016356	-1.49473680	3.05588434	3	119	Ru
-1.37062182	-1.49678994	2.78480418	3	120	Ru
2.34275979	-0.00001996	3.82485857	3	121	Ru
0.61335501	-0.00010994	4.51508213	3	122	Ru
-1.20809403	-0.00015645	4.30577396	3	123	Ru
2.28749283	0.99818716	3.79028432	3	124	Ru
0.66799429	0.91789257	4.04414047	3	125	Ru
-1.18944727	1.02196436	4.33345011	3	126	Ru
2.28521596	-0.99812180	3.78801278	3	127	Ru
0.66860148	-0.91871096	4.04410793	3	128	Ru
-1.18922338	-1.02205179	4.33384649	3	129	Ru
2.24363758	-2.00027109	3.61908448	3	130	Ru
0.62332558	-2.00051529	4.16237445	3	131	Ru
-1.18316860	-1.99982881	4.17294600	3	132	Ru
-1.90696832	0.51382191	3.77394636	3	133	Ru
-0.27815485	0.49947367	4.26061590	3	134	Ru
1.57533932	0.50576806	4.40396551	3	135	Ru
-1.98238694	1.51025982	3.74538504	3	136	Ru
-0.24448201	1.49653103	4.20402587	3	137	Ru
1.52043205	1.49787635	4.20574220	3	138	Ru
-1.90653356	-0.51407552	3.77332043	3	139	Ru
-0.27769382	-0.49980158	4.26054988	3	140	Ru
1.57528500	-0.50610045	4.40417277	3	141	Ru
-1.98351537	-1.50982430	3.74578614	3	142	Ru
-0.24383679	-1.49651075	4.20376613	3	143	Ru

1.52078605	-1.49867090	4.20647505	3	144	Ru

Penetration throughout 2vacancy

0.86139469	-0.00000385	0.23152296	2	1	O
0.86091976	-0.00000129	-0.23152296	1	2	C
-2.36165394	-0.08762963	-0.24235044	1	3	C
-1.18487204	-0.09648513	-0.16996554	1	4	C
-0.60778453	-0.10369563	-0.16043066	1	5	C
2.25807486	-0.08323901	-0.30017380	1	6	C
-2.35147293	0.90604234	-0.17191287	1	7	C
-1.18216426	0.89847310	-0.10696408	1	8	C
-0.59945064	0.89538015	-0.06463248	1	9	C
2.26699954	0.90898012	-0.18393654	1	10	C
1.15922281	0.91719492	-0.00222259	1	11	C
0.57374539	0.91727465	-0.00201467	1	12	C
-2.35144857	-1.08825871	-0.21784510	1	13	C
-1.18714199	-1.09361086	-0.18374342	1	14	C
-0.60636666	-1.09838522	-0.20255503	1	15	C
2.26668042	-1.08272921	-0.24343325	1	16	C
1.12382783	-1.09473642	-0.28779444	1	17	C
0.53775711	-1.09729088	-0.27802172	1	18	C
-2.33940776	-2.08906523	-0.15884477	1	19	C
-1.18703848	-2.09641414	-0.12206845	1	20	C
-0.60824138	-2.10048402	-0.10739935	1	21	C
2.28464175	-2.08389660	-0.15381894	1	22	C
1.12972343	-2.08108810	-0.08812822	1	23	C
0.55110977	-2.08697357	-0.08959608	1	24	C
1.95775419	0.41700072	-0.27747562	1	25	C
1.37427210	0.46737083	-0.27915937	1	26	C
0.26079493	0.41020094	-0.00186356	1	27	C
-2.05986984	0.40682066	-0.18946620	1	28	C
-1.47925489	0.40319234	-0.14802667	1	29	C
-0.31051508	0.37998875	-0.06424317	1	30	C
1.99841464	1.41718437	-0.12391637	1	31	C
1.42857931	1.42518546	-0.04160142	1	32	C
0.26954249	1.40824896	-0.04366586	1	33	C
-2.05553199	1.40485458	-0.14301328	1	34	C
-1.47447378	1.40086472	-0.11876260	1	35	C
-0.31395442	1.39950097	-0.06240096	1	36	C
1.95998388	-0.58464988	-0.30942398	1	37	C
1.38130193	-0.59386651	-0.34590265	1	38	C
0.25662176	-0.61100027	-0.34404656	1	39	C
-2.06227062	-0.58873113	-0.22357406	1	40	C
-1.48158333	-0.59348978	-0.19984086	1	41	C
-0.30729165	-0.59621301	-0.24516789	1	42	C
1.99003864	-1.58501213	-0.19163520	1	43	C
1.41296421	-1.58805184	-0.18964471	1	44	C
0.25633165	-1.59443903	-0.16567619	1	45	C
-2.05525608	-1.58700620	-0.17566120	1	46	C
-1.47641021	-1.59295037	-0.15737990	1	47	C
-0.32077773	-1.59846576	-0.15948675	1	48	C
-2.31317667	0.00000226	1.04123872	3	49	Ru
-0.57879212	-0.00000193	1.04164328	3	50	Ru
1.15528706	0.00000024	1.04632471	3	51	Ru
-2.31317725	0.99999828	1.04123893	3	52	Ru
-0.57879220	1.00000221	1.04164330	3	53	Ru
1.15528699	0.99999983	1.04632457	3	54	Ru
-2.31322024	-1.00000043	1.04123989	3	55	Ru
-0.57879492	-0.99999972	1.04164338	3	56	Ru
1.15528760	-0.99999984	1.04632454	3	57	Ru
-2.31322033	-1.99999946	1.04123964	3	58	Ru
-0.57879514	-1.99999991	1.04164332	3	59	Ru

1.15528768	-1.99999970	1.04632490	3	60	Ru
2.01826631	0.50000040	1.04156336	3	61	Ru
0.28627502	0.50000014	1.04304188	3	62	Ru
-1.44460545	0.49999992	1.04609833	3	63	Ru
2.01827301	1.49998902	1.04155385	3	64	Ru
0.28627254	1.50000473	1.04304130	3	65	Ru
-1.44461139	1.50000017	1.04608177	3	66	Ru
2.01826668	-0.50000070	1.04156333	3	67	Ru
0.28627274	-0.50000427	1.04304119	3	68	Ru
-1.44461172	-0.49999970	1.04608207	3	69	Ru
2.01826776	-1.49999996	1.04156355	3	70	Ru
0.28627130	-1.49999983	1.04304054	3	71	Ru
-1.44460924	-1.49999988	1.04608250	3	72	Ru
2.31592695	0.00000009	2.00527822	3	73	Ru
0.58417204	-0.00000007	2.00632071	3	74	Ru
-1.14788682	-0.00000005	2.00559252	3	75	Ru
2.31592656	1.00000035	2.00527828	3	76	Ru
0.58417173	1.00000019	2.00632062	3	77	Ru
-1.14788711	1.00000030	2.00559254	3	78	Ru
2.31592702	-0.99999984	2.00527836	3	79	Ru
0.58417164	-0.99999975	2.00632074	3	80	Ru
-1.14788711	-0.99999985	2.00559240	3	81	Ru
2.31592705	-1.99999996	2.00527821	3	82	Ru
0.58417122	-2.00000038	2.00632087	3	83	Ru
-1.14788755	-2.00000025	2.00559248	3	84	Ru
-2.01489331	0.49999985	2.00616344	3	85	Ru
-0.28261107	0.49999990	2.00576107	3	86	Ru
1.45230538	0.49999985	2.00586814	3	87	Ru
-2.01489282	1.50000051	2.00616320	3	88	Ru
-0.28261044	1.50000015	2.00576098	3	89	Ru
1.45230566	1.49999982	2.00586787	3	90	Ru
-2.01489304	-0.50000015	2.00616355	3	91	Ru
-0.28261092	-0.49999980	2.00576091	3	92	Ru
1.45230547	-0.49999966	2.00586789	3	93	Ru
-2.01489239	-1.50000011	2.00616355	3	94	Ru
-0.28261066	-1.49999990	2.00576075	3	95	Ru
1.45230600	-1.50000000	2.00586772	3	96	Ru
-2.31268477	-0.00000019	2.99128225	3	97	Ru
-0.58078260	-0.00000081	3.00213715	3	98	Ru
1.15389758	-0.00000035	2.99982477	3	99	Ru
-2.31268513	0.99999996	2.99128237	3	100	Ru
-0.58078277	1.00000058	3.00213714	3	101	Ru
1.15389798	1.00000028	2.99982446	3	102	Ru
-2.31268425	-1.00000005	2.99128219	3	103	Ru
-0.58078259	-1.00000067	3.00213698	3	104	Ru
1.15389763	-1.00000029	2.99982460	3	105	Ru
-2.31268445	-2.00000008	2.99128234	3	106	Ru
-0.58078260	-1.99999977	3.00213687	3	107	Ru
1.15389731	-2.00000003	2.99982442	3	108	Ru
2.01934772	0.50000036	2.99815968	3	109	Ru
0.28729638	0.49999979	2.99234919	3	110	Ru
-1.44342084	0.49999998	2.99519965	3	111	Ru
2.01934735	1.49999855	2.99815980	3	112	Ru
0.28729640	1.49999989	2.99234921	3	113	Ru
-1.44342047	1.49999952	2.99519973	3	114	Ru
2.01934770	-0.50000008	2.99815955	3	115	Ru
0.28729654	-0.49999996	2.99234912	3	116	Ru
-1.44342042	-0.50000038	2.99519954	3	117	Ru
2.01934748	-1.49999931	2.99815948	3	118	Ru
0.28729668	-1.50000023	2.99234919	3	119	Ru
-1.44342029	-1.49999968	2.99519937	3	120	Ru
2.31018337	-0.00000025	3.97747823	3	121	Ru

0.57746189	-0.00000040	3.97629485	3	122	Ru
-1.15795492	-0.00000018	3.97952317	3	123	Ru
2.31018323	0.99999983	3.97747793	3	124	Ru
0.57743737	0.99998965	3.97628204	3	125	Ru
-1.15795502	0.99999962	3.97952313	3	126	Ru
2.31018351	-1.00000043	3.97747806	3	127	Ru
0.57741328	-1.00000038	3.97626913	3	128	Ru
-1.15795487	-0.99999996	3.97952305	3	129	Ru
2.31018327	-2.00000030	3.97747806	3	130	Ru
0.57743731	-2.00001025	3.97628219	3	131	Ru
-1.15795515	-2.00000048	3.97952297	3	132	Ru
-2.02178838	0.49999975	3.97571631	3	133	Ru
-0.28901724	0.50000010	3.97942356	3	134	Ru
1.44083223	0.49999960	3.98029309	3	135	Ru
-2.02178844	1.49999996	3.97571628	3	136	Ru
-0.28901724	1.49999935	3.97942354	3	137	Ru
1.44083277	1.49999993	3.98029303	3	138	Ru
-2.02178840	-0.50000020	3.97571614	3	139	Ru
-0.28901733	-0.49999979	3.97942334	3	140	Ru
1.44083200	-0.50000021	3.98029292	3	141	Ru
-2.02178874	-1.50000039	3.97571609	3	142	Ru
-0.28901718	-1.50000005	3.97942311	3	143	Ru
1.44083198	-1.50000029	3.98029287	3	144	Ru

Penetration throughout 4 vacancy

0.58800000	0.00000000	0.23152296	2	1	O
0.58800000	0.00000000	-0.23152296	1	2	C
-2.29513521	0.00162886	-0.00164524	1	3	C
-1.08500566	-0.00425167	0.00037259	1	4	C
-0.45629516	-0.02024968	0.00524386	1	5	C
2.33462125	0.01401771	-0.00274775	1	6	C
-2.30477139	1.00812325	-0.00058585	1	7	C
-1.14048276	0.99588160	-0.00056643	1	8	C
-0.55386270	0.99315533	-0.00132640	1	9	C
2.31784579	1.02137166	-0.00176574	1	10	C
1.16000000	1.00000000	0.00000000	1	11	C
0.58000000	1.00000000	0.00000000	1	12	C
-2.30121769	-0.98270430	-0.00122600	1	13	C
-1.13131401	-0.99856789	-0.00153313	1	14	C
-0.55121851	-1.01157123	-0.00149912	1	15	C
2.31252637	-0.97167287	-0.00126826	1	16	C
1.08706442	-0.89246975	0.00586897	1	17	C
0.46477617	-0.94074343	0.00611795	1	18	C
-2.31517378	-1.98366890	-0.00029760	1	19	C
-1.15620943	-2.00256129	-0.00142369	1	20	C
-0.57770607	-2.01248847	-0.00274299	1	21	C
2.29944528	-1.96951049	-0.00046912	1	22	C
1.15187461	-1.96183720	-0.00151177	1	23	C
0.57833293	-1.98145265	-0.00262143	1	24	C
2.03906616	0.51321828	-0.00277299	1	25	C
1.47868624	0.48548004	0.00030531	1	26	C
-2.02000000	0.50000000	0.00000000	1	27	C
-1.41508612	0.49029059	0.00012140	1	28	C
-0.23263695	0.52401534	0.00301771	1	29	C
2.02054622	1.52199181	-0.00131391	1	30	C
1.44217630	1.52393123	-0.00177936	1	31	C
0.30199553	1.50048902	-0.00291919	1	32	C
-2.02035640	1.51053861	-0.00022321	1	33	C
-1.44034026	1.49850690	-0.00058521	1	34	C
-0.27995341	1.50044732	-0.00269201	1	35	C
2.01998204	-0.46863947	-0.00199929	1	36	C
1.45119246	-0.41738645	0.00323628	1	37	C

-1.99264161	-0.49200261	-0.00125040	1	38	C
-1.40534952	-0.49275841	-0.00072269	1	39	C
-0.17620474	-0.57604594	0.00659547	1	40	C
2.00083335	-1.45857529	-0.00052666	1	41	C
1.41081453	-1.43087628	-0.00010948	1	42	C
0.27678670	-1.48610858	-0.00217146	1	43	C
-2.01644879	-1.48765418	-0.00071023	1	44	C
-1.43510523	-1.49534231	-0.00130045	1	45	C
-0.29459063	-1.52214659	-0.00302699	1	46	C
-2.31317667	0.00000226	1.04123872	3	47	Ru
-0.57879212	-0.00000193	1.04164328	3	48	Ru
1.15528706	0.00000024	1.04632471	3	49	Ru
-2.31317725	0.99999828	1.04123893	3	50	Ru
-0.57879220	1.00000221	1.04164330	3	51	Ru
1.15528699	0.99999983	1.04632457	3	52	Ru
-2.31322024	-1.00000043	1.04123989	3	53	Ru
-0.57879492	-0.99999972	1.04164338	3	54	Ru
1.15528760	-0.99999984	1.04632454	3	55	Ru
-2.31322033	-1.99999946	1.04123964	3	56	Ru
-0.57879514	-1.99999991	1.04164332	3	57	Ru
1.15528768	-1.99999970	1.04632490	3	58	Ru
2.01826631	0.50000040	1.04156336	3	59	Ru
0.28627502	0.50000014	1.04304188	3	60	Ru
-1.44460545	0.49999992	1.04609833	3	61	Ru
2.01827301	1.49998902	1.04155385	3	62	Ru
0.28627254	1.50000473	1.04304130	3	63	Ru
-1.44461139	1.50000017	1.04608177	3	64	Ru
2.01826668	-0.50000070	1.04156333	3	65	Ru
0.28627274	-0.50000427	1.04304119	3	66	Ru
-1.44461172	-0.49999970	1.04608207	3	67	Ru
2.01826776	-1.49999996	1.04156355	3	68	Ru
0.28627130	-1.49999983	1.04304054	3	69	Ru
-1.44460924	-1.49999988	1.04608250	3	70	Ru
2.31592695	0.00000009	2.00527822	3	71	Ru
0.58417204	-0.00000007	2.00632071	3	72	Ru
-1.14788682	-0.00000005	2.00559252	3	73	Ru
2.31592656	1.00000035	2.00527828	3	74	Ru
0.58417173	1.00000019	2.00632062	3	75	Ru
-1.14788711	1.00000030	2.00559254	3	76	Ru
2.31592702	-0.99999984	2.00527836	3	77	Ru
0.58417164	-0.99999975	2.00632074	3	78	Ru
-1.14788711	-0.99999985	2.00559240	3	79	Ru
2.31592705	-1.99999996	2.00527821	3	80	Ru
0.58417122	-2.00000038	2.00632087	3	81	Ru
-1.14788755	-2.00000025	2.00559248	3	82	Ru
-2.01489331	0.49999985	2.00616344	3	83	Ru
-0.28261107	0.49999990	2.00576107	3	84	Ru
1.45230538	0.49999985	2.00586814	3	85	Ru
-2.01489282	1.50000051	2.00616320	3	86	Ru
-0.28261044	1.50000015	2.00576098	3	87	Ru
1.45230566	1.49999982	2.00586787	3	88	Ru
-2.01489304	-0.50000015	2.00616355	3	89	Ru
-0.28261092	-0.49999980	2.00576091	3	90	Ru
1.45230547	-0.49999966	2.00586789	3	91	Ru
-2.01489239	-1.50000011	2.00616355	3	92	Ru
-0.28261066	-1.49999990	2.00576075	3	93	Ru
1.45230600	-1.50000000	2.00586772	3	94	Ru
-2.31268477	-0.00000019	2.99128225	3	95	Ru
-0.58078260	-0.00000081	3.00213715	3	96	Ru
1.15389758	-0.00000035	2.99982477	3	97	Ru
-2.31268513	0.99999996	2.99128237	3	98	Ru
-0.58078277	1.00000058	3.00213714	3	99	Ru

1.15389798	1.00000028	2.99982446	3	100	Ru
-2.31268425	-1.00000005	2.99128219	3	101	Ru
-0.58078259	-1.00000067	3.00213698	3	102	Ru
1.15389763	-1.00000029	2.99982460	3	103	Ru
-2.31268445	-2.00000008	2.99128234	3	104	Ru
-0.58078260	-1.99999977	3.00213687	3	105	Ru
1.15389731	-2.00000003	2.99982442	3	106	Ru
2.01934772	0.50000036	2.99815968	3	107	Ru
0.28729638	0.49999979	2.99234919	3	108	Ru
-1.44342084	0.49999998	2.99519965	3	109	Ru
2.01934735	1.49999855	2.99815980	3	110	Ru
0.28729640	1.49999989	2.99234921	3	111	Ru
-1.44342047	1.49999952	2.99519973	3	112	Ru
2.01934770	-0.50000008	2.99815955	3	113	Ru
0.28729654	-0.49999996	2.99234912	3	114	Ru
-1.44342042	-0.50000038	2.99519954	3	115	Ru
2.01934748	-1.49999931	2.99815948	3	116	Ru
0.28729668	-1.50000023	2.99234919	3	117	Ru
-1.44342029	-1.49999968	2.99519937	3	118	Ru
2.31018337	-0.00000025	3.97747823	3	119	Ru
0.57746189	-0.00000040	3.97629485	3	120	Ru
-1.15795492	-0.00000018	3.97952317	3	121	Ru
2.31018323	0.99999983	3.97747793	3	122	Ru
0.57743737	0.99998965	3.97628204	3	123	Ru
-1.15795502	0.99999962	3.97952313	3	124	Ru
2.31018351	-1.00000043	3.97747806	3	125	Ru
0.57741328	-1.00000038	3.97626913	3	126	Ru
-1.15795487	-0.99999996	3.97952305	3	127	Ru
2.31018327	-2.00000030	3.97747806	3	128	Ru
0.57743731	-2.00001025	3.97628219	3	129	Ru
-1.15795515	-2.00000048	3.97952297	3	130	Ru
-2.02178838	0.49999975	3.97571631	3	131	Ru
-0.28901724	0.50000010	3.97942356	3	132	Ru
1.44083223	0.49999960	3.98029309	3	133	Ru
-2.02178844	1.49999996	3.97571628	3	134	Ru
-0.28901724	1.49999935	3.97942354	3	135	Ru
1.44083277	1.49999993	3.98029303	3	136	Ru
-2.02178840	-0.50000020	3.97571614	3	137	Ru
-0.28901733	-0.49999979	3.97942334	3	138	Ru
1.44083200	-0.50000021	3.98029292	3	139	Ru
-2.02178874	-1.50000039	3.97571609	3	140	Ru
-0.28901718	-1.50000005	3.97942311	3	141	Ru
1.44083198	-1.50000029	3.98029287	3	142	Ru

Adsorption on 4vacancy

1)

-0.46062735	-0.02717188	-1.05587244	2	1	O
-0.45833536	-0.02601916	-1.52412567	1	2	C
-2.30049437	0.00361405	0.02948203	1	3	C
-1.08792427	-0.00742862	0.01942439	1	4	C
-0.47556534	-0.01460755	0.03383222	1	5	C
2.31752322	0.01844475	0.06282838	1	6	C
-2.30617421	1.00954734	-0.00357418	1	7	C
-1.14224666	0.99605444	-0.01800120	1	8	C
-0.55987218	0.99690204	-0.01918158	1	9	C
2.31481191	1.01900508	-0.00843097	1	10	C
1.16000000	1.00000000	0.00000000	1	11	C
0.58000000	1.00000000	0.00000000	1	12	C
-2.30641054	-0.98500465	0.01066987	1	13	C
-1.12767050	-0.99644477	0.02125212	1	14	C
-0.54471306	-1.00826861	0.04963506	1	15	C
2.30733448	-0.97412380	0.02230170	1	16	C

1.08295230	-0.93352169	0.03707712	1	17	C
0.46477617	-0.94074343	0.00611795	1	18	C
-2.31517378	-1.98366890	-0.00029760	1	19	C
-1.15620943	-2.00256129	-0.00142369	1	20	C
-0.57770607	-2.01248847	-0.00274299	1	21	C
2.29863426	-1.96883582	0.00020287	1	22	C
1.15187461	-1.96183720	-0.00151177	1	23	C
0.57469394	-1.98294023	-0.01961098	1	24	C
2.02865482	0.52346946	0.04209837	1	25	C
1.46569806	0.53877375	0.11257334	1	26	C
-2.02000000	0.50000000	0.00000000	1	27	C
-1.41945770	0.48990289	0.00749467	1	28	C
-0.23263695	0.52401534	0.00301771	1	29	C
2.02054622	1.52199181	-0.00131391	1	30	C
1.44217630	1.52393123	-0.00177936	1	31	C
0.30199553	1.50048902	-0.00291919	1	32	C
-2.02035640	1.51053861	-0.00022321	1	33	C
-1.44034026	1.49850690	-0.00058521	1	34	C
-0.28066831	1.50178531	-0.00591255	1	35	C
2.00914834	-0.47964437	0.07014223	1	36	C
1.43052844	-0.47276606	0.10821964	1	37	C
-1.99749453	-0.49220475	0.01465428	1	38	C
-1.41343676	-0.49433440	0.02039133	1	39	C
-0.15156852	-0.56294912	0.07167342	1	40	C
1.99744550	-1.46168948	0.01966845	1	41	C
1.40392138	-1.44283829	0.01278561	1	42	C
0.27142526	-1.49071841	-0.00227818	1	43	C
-2.01830809	-1.48482129	-0.00268029	1	44	C
-1.43516439	-1.49423164	0.01200870	1	45	C
-0.29581456	-1.52101216	0.00722942	1	46	C
-2.31317667	0.00000226	1.04123872	3	47	Ru
-0.54343650	0.01418162	1.06029564	3	48	Ru
1.14320859	0.03547405	0.68386325	3	49	Ru
-2.31798879	0.99538643	1.13262119	3	50	Ru
-0.54744826	0.98082858	1.13829917	3	51	Ru
1.11574536	0.94761636	1.13656094	3	52	Ru
-2.31193306	-0.99773066	1.13333626	3	53	Ru
-0.56711527	-0.99126287	1.11609418	3	54	Ru
1.14833495	-0.96354257	1.07396170	3	55	Ru
-2.31411586	-2.00324875	1.10824845	3	56	Ru
-0.57267042	-1.99993646	1.12755694	3	57	Ru
1.15088179	-2.00718568	1.08802283	3	58	Ru
1.99279634	0.48196618	1.15604228	3	59	Ru
0.28446617	0.54748755	0.61233988	3	60	Ru
-1.44451833	0.50248794	1.09597849	3	61	Ru
2.00846622	1.48641570	1.09160663	3	62	Ru
0.28797351	1.47925372	1.11878319	3	63	Ru
-1.43132472	1.49612375	1.10590764	3	64	Ru
2.01826668	-0.50000070	1.04156333	3	65	Ru
0.28526885	-0.49578309	0.84810613	3	66	Ru
-1.43593584	-0.49707888	1.11268398	3	67	Ru
2.01945062	-1.50441632	1.09739906	3	68	Ru
0.29551133	-1.49082948	1.13805268	3	69	Ru
-1.44105069	-1.50235464	1.09382864	3	70	Ru
2.31458471	-0.00394228	1.99725089	3	71	Ru
0.58087458	0.03111780	1.68277394	3	72	Ru
-1.14098469	0.00066043	1.94951687	3	73	Ru
2.30183798	0.99902431	2.02198946	3	74	Ru
0.57970707	0.98118878	2.07625112	3	75	Ru
-1.14767799	0.99349005	2.01752747	3	76	Ru
2.29735070	-0.99423473	2.00411790	3	77	Ru
0.58116186	-0.96996751	2.06253689	3	78	Ru

-1.14666599	-0.99170762	2.03125362	3	79	Ru
2.29857414	-1.99683539	2.04289357	3	80	Ru
0.58308848	-1.99640561	2.03780942	3	81	Ru
-1.14981107	-1.99857966	2.03047844	3	82	Ru
-2.01994707	0.49523623	2.03645264	3	83	Ru
-0.27266482	0.48988672	2.09077955	3	84	Ru
1.42241054	0.48410364	2.08321006	3	85	Ru
-2.02314899	1.50111036	2.04761979	3	86	Ru
-0.28622955	1.49908749	2.00011845	3	87	Ru
1.43778145	1.49855069	1.96670403	3	88	Ru
-2.01676790	-0.49598556	2.04339916	3	89	Ru
-0.27170472	-0.48563334	2.07277570	3	90	Ru
1.41899593	-0.48048967	2.05026878	3	91	Ru
-2.02499748	-1.49971022	2.02974652	3	92	Ru
-0.28610878	-1.49556284	2.00300361	3	93	Ru
1.43459418	-1.48997566	1.95106147	3	94	Ru
-2.30908862	0.00070374	2.98129010	3	95	Ru
-0.57994961	-0.00051103	2.97128015	3	96	Ru
1.16151934	0.00064042	3.04324670	3	97	Ru
-2.30989134	0.99980075	2.94883466	3	98	Ru
-0.57549621	1.00484203	2.97635231	3	99	Ru
1.15871356	1.00747671	2.94373334	3	100	Ru
-2.31225667	-1.00076551	2.94120750	3	101	Ru
-0.57261549	-1.00266033	2.95591669	3	102	Ru
1.15977787	-1.00334846	2.93143386	3	103	Ru
-2.31096745	-1.99928101	2.94623709	3	104	Ru
-0.57693610	-1.99756939	3.06253896	3	105	Ru
1.15226418	-1.99782009	3.00674399	3	106	Ru
2.02604095	0.49788788	2.92824929	3	107	Ru
0.29828307	0.49532165	2.96766245	3	108	Ru
-1.44002844	0.49903094	2.95113625	3	109	Ru
2.02129572	1.50023318	2.99274464	3	110	Ru
0.28224278	1.50526926	2.91110421	3	111	Ru
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0.57937511	1.00110766	3.86425547	3	123	Ru
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-1.15577853	-0.99974104	3.89286429	3	127	Ru
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0.58008411	-1.99920417	3.88545457	3	129	Ru
-1.15447246	-1.99936225	3.91762713	3	130	Ru
-2.02415748	0.49880254	3.88327597	3	131	Ru
-0.28922115	0.49801045	3.89266842	3	132	Ru
1.44463255	0.50067753	3.90225483	3	133	Ru
-2.02027837	1.49972413	3.86731296	3	134	Ru
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0.58894576	-1.99315095	4.10695231	3	129	Ru
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-1.97736321	0.48171436	3.83512006	3	131	Ru
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-1.96590160	1.50270013	3.88934148	3	134	Ru
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-0.21518748	0.46000580	3.98982204	3	132	Ru
1.48712330	0.50296370	4.37488486	3	133	Ru
-1.93066833	1.49678524	3.87792110	3	134	Ru
-0.23758526	1.47600999	4.06917552	3	135	Ru
1.51517115	1.48729456	4.22284156	3	136	Ru
-2.05632945	-0.46423413	4.11761819	3	137	Ru
-0.17779530	-0.60487790	3.83406608	3	138	Ru
1.46054064	-0.52228737	4.43429556	3	139	Ru
-1.88759303	-1.45955299	3.81697326	3	140	Ru
-0.22147632	-1.49774933	4.23328695	3	141	Ru
1.49057270	-1.51531925	4.25924333	3	142	Ru

Pure graphene
Adsorption 2vacancy

-0.60221210	0.00000219	-1.06137107	2	1	O
-0.61366003	0.00001315	-1.52422274	1	2	C
-2.29621243	0.00000725	0.02453940	1	3	C
-1.17685451	0.00000785	0.02038336	1	4	C
-0.61860047	0.00000959	0.04622199	1	5	C
2.34531813	0.00001015	0.05494882	1	6	C
-2.31755574	1.00252438	0.02632000	1	7	C
-1.15510812	1.00241530	0.01898739	1	8	C
-0.57622120	0.99396045	0.03425976	1	9	C
2.30374575	0.99445350	0.04953048	1	10	C
1.15592785	0.90820136	0.07801648	1	11	C
0.57090371	0.90732838	0.06962142	1	12	C
-2.31755959	-1.00250791	0.02632921	1	13	C
-1.15511030	-1.00239936	0.01899638	1	14	C
-0.57622614	-0.99394418	0.03426183	1	15	C
2.30374444	-0.99443678	0.04953108	1	16	C
1.15592750	-0.90818487	0.07800903	1	17	C
0.57090278	-0.90731079	0.06961568	1	18	C
-2.32624148	-1.99999318	0.02617439	1	19	C
-1.14632926	-1.99999010	0.01823890	1	20	C
-0.56576680	-1.99998298	0.02871239	1	21	C
2.29324247	-1.99999033	0.04210474	1	22	C
1.14934678	-1.99999281	0.06977959	1	23	C
0.57734338	-1.99999206	0.06245111	1	24	C
2.03120773	0.48105521	0.06644703	1	25	C
1.47009392	0.39500817	0.08149196	1	26	C
0.25704597	0.39309451	0.06446336	1	27	C
-2.02058243	0.50815977	0.01528317	1	28	C
-1.45231471	0.50803443	0.01274561	1	29	C
-0.30407814	0.48035282	0.04899119	1	30	C
2.00606744	1.48880975	0.05513557	1	31	C
1.42829678	1.46173693	0.07046375	1	32	C
0.29867766	1.46112896	0.05758251	1	33	C
-2.02720400	1.50218903	0.01993249	1	34	C
-1.44533242	1.50213830	0.01602831	1	35	C
-0.27884910	1.48850801	0.03905216	1	36	C
2.03120699	-0.48103897	0.06644533	1	37	C
1.47009300	-0.39498959	0.08148864	1	38	C
0.25704581	-0.39307366	0.06446178	1	39	C

-2.02058317	-0.50814563	0.01528836	1	40	C
-1.45231435	-0.50801523	0.01275097	1	41	C
-0.30407814	-0.48033583	0.04899223	1	42	C
2.00606665	-1.48879296	0.05513323	1	43	C
1.42829653	-1.46172114	0.07045769	1	44	C
0.29867808	-1.46111268	0.05757666	1	45	C
-2.02720478	-1.50217473	0.01994331	1	46	C
-1.44533286	-1.50212230	0.01603969	1	47	C
-0.27884862	-1.48848876	0.03904917	1	48	C

Adsorption 4vacancy

-0.46368677	-0.02829881	-1.07420958	2	1	O
-0.46017981	-0.03085702	-1.53707818	1	2	C
-2.27836067	0.01128070	0.02841500	1	3	C
-1.04354599	0.00942477	0.01766406	1	4	C
-0.38603721	0.00902909	0.02181529	1	5	C
2.34347188	0.01107476	0.03801895	1	6	C
-2.30544418	0.99729874	0.00986999	1	7	C
-1.11744717	1.00423342	-0.00078486	1	8	C
-0.53317565	1.00419689	-0.00065764	1	9	C
2.29935941	0.99099572	0.01765140	1	10	C
1.07147751	0.86973708	0.01981652	1	11	C
0.46604833	0.92894842	0.01217006	1	12	C
-2.30600633	-0.97465693	0.02096914	1	13	C
-1.11772711	-0.98465434	0.01385213	1	14	C
-0.53364611	-0.98568699	0.01375997	1	15	C
2.29794948	-0.96856511	0.02722618	1	16	C
1.06926700	-0.84474056	0.02647085	1	17	C
0.46339317	-0.90649540	0.02111076	1	18	C
-2.32862722	-1.98864066	0.00446000	1	19	C
-1.16055553	-1.98961967	-0.00266459	1	20	C
-0.58181604	-1.99044025	-0.00280645	1	21	C
2.27468950	-1.98853965	0.00932870	1	22	C
1.13979645	-1.98917653	0.01444204	1	23	C
0.56698463	-1.98942187	0.00856912	1	24	C
2.01340218	0.48388930	0.03158603	1	25	C
1.43127345	0.35974048	0.02996135	1	26	C
-1.98180445	0.50590278	0.01499221	1	27	C
-1.38261298	0.49604947	0.00995945	1	28	C
-0.13453702	0.57068398	0.01048774	1	29	C
1.98688507	1.48937792	0.01203020	1	30	C
1.39932776	1.45995049	0.01534690	1	31	C
0.28190199	1.49548367	0.00332366	1	32	C
-2.02509102	1.50715015	0.00068282	1	33	C
-1.43737941	1.50343681	-0.00384594	1	34	C
-0.28916518	1.52165447	-0.00428384	1	35	C
2.01191392	-0.46102527	0.03796796	1	36	C
1.42977169	-0.33555121	0.03382821	1	37	C
-1.98189823	-0.48414356	0.02400405	1	38	C
-1.38286415	-0.47651344	0.02003662	1	39	C
-0.13423221	-0.55229583	0.02062234	1	40	C
1.98566205	-1.46677640	0.01817869	1	41	C
1.39833497	-1.43668291	0.01986910	1	42	C
0.28180834	-1.47494891	0.01112605	1	43	C
-2.02578959	-1.48478148	0.00886774	1	44	C
-1.43800939	-1.48288717	0.00579642	1	45	C
-0.28898177	-1.50286927	0.00598723	1	46	C