

# Supplementary Materials

Brief Report

## Non-Monotonic Trends of Hydrogen Adsorption on Single Atom Doped g-C<sub>3</sub>N<sub>4</sub>

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### Optimized Geometries (Format: VASP POSCAR)

#### Ir doped g-C<sub>3</sub>N<sub>4</sub>

C N Ir

```
1.0000000000000000
14.3700000000000010 0.0000000000000000 0.0000000000000000
-7.1850000000000005 12.4447860000000006 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000
```

C N Ir

27 36 1

Direct

```
0.1173694894088664 0.0577691486677136 0.5186221388923007
0.2717565146525349 0.0571953027396645 0.4843050146708586
0.2712637543777122 0.2129122370087843 0.4935150208389599
0.1161829343147511 0.3937978350352118 0.4787748834081970
0.2672765285966087 0.3838764906606588 0.4978645811515318
0.2714881974131833 0.5466097757810675 0.5199472474298001
0.1168745405721343 0.7246511536625813 0.5007272897527405
0.2738641966931059 0.7271219588232819 0.5231620344127418
0.2741220512429866 0.8814749925869213 0.4875184870585897
```

0.4515385329418128 0.0613376476341158 0.4863210447991867  
0.6075284619320928 0.0608470464391361 0.4955718333502590  
0.6067935870674479 0.2155131031235990 0.5229442404399656  
0.4475570163418243 0.3907945144358559 0.5004009466418641  
0.6077617017753848 0.3951584213901522 0.5227835487257166  
0.6061466721461372 0.5512520070667730 0.4961373201404707  
0.4536644592768286 0.7279340821332221 0.5229839552383547  
0.6167303744386414 0.7328522388496866 0.4857633193529518  
0.6081390043023049 0.8856374627309570 0.4897846591418007  
0.7840134807581967 0.0599876672338432 0.4937427705154505  
0.9403135367175331 0.0606458187431810 0.5173105340941869  
0.9406661433763830 0.2155650752877220 0.4807510807354146  
0.7846413682962965 0.3916941731756902 0.5225947654773870  
0.9384473491917644 0.3926777872392687 0.4826171950676433  
0.9398141321771092 0.5489045054933096 0.4998925468138400  
0.7875153158487731 0.7292401401822695 0.4769464305028877  
0.9412183526165698 0.7261025033904973 0.4983031640060619  
0.9403788800455500 0.8818774535455902 0.5166293029714636  
0.9993507423387523 0.0004136256258220 0.5226679445112767  
0.1714455080263116 0.1646510034233011 0.5277174316720011  
0.1677339685974086 0.0015381659095091 0.5064334857010924  
0.3224466233713321 0.1622305535823299 0.4630421438337890  
0.9990191018479326 0.3344414538005274 0.4761052448983551  
0.1697081738449096 0.4999713187637394 0.4942226717702087  
0.1697411323746489 0.3403452818063799 0.4636478740231239  
0.3164170505077785 0.4843877344107386 0.5410007869610552  
-0.0002721899227648 0.6666913236609273 0.4998358464166244  
0.1684828927754454 0.8257139823531161 0.4681985590573017  
0.1669509374018609 0.6733127321099923 0.5334053667623276  
0.3298728654945873 0.8330134991844070 0.5104062632157952  
0.3323860975299074 -0.0004279241644989 0.4824053728861483  
0.4995171230988003 0.1642808067335670 0.5117445232157761

0.5063049202110841 0.0114708153499808 0.4635537197760159  
 0.6591014896274975 0.1596697761942945 0.5308424669366770  
 0.3277406082874152 0.3286550752018471 0.4915068862491292  
 0.5028982249443121 0.4891359038097764 0.4468150811870255  
 0.4988984427076068 0.3413272834663035 0.5355402195529835  
 0.6642448222247638 0.4987987648294058 0.5083907303720776  
 0.3348798367800480 0.6658845799776211 0.5269276362460007  
 0.5052326922057815 0.8337065867864970 0.5160019052027901  
 0.5159953019696903 0.6798983559548251 0.5290492070009364  
 0.6585572191213112 0.8338775301752088 0.4586445180262209  
 0.6663099716565596 0.0016552032461224 0.4919034097459342  
 0.8351713552461790 0.1609030051681768 0.4612372270382523  
 0.8326644594223059 0.0082943005071793 0.5274781098922570  
 0.9961218295235539 0.1670596522773408 0.5037123410135337  
 0.6666468926489550 0.3328433819789164 0.5282648478433242  
 0.8402667883150490 0.4993303330698388 0.5346039227249574  
 0.8352670704304663 0.3363081948626457 0.5061406998999797  
 0.9894978054929318 0.4985656411100748 0.4650452793180526  
 0.6712266198665555 0.6725786762237890 0.4746257386170740  
 0.8369642226594050 0.8344246932177358 0.4954300060084746  
 0.8417801614218736 0.6764018001415788 0.4625876331411959  
 0.9910324961790494 0.8259970259948399 0.5328828459887426  
 0.4732308600563841 0.5320054107661534 0.5661027774604719

**Os doped g-C<sub>3</sub>N<sub>4</sub>**

C N Os

1.0000000000000000  
 14.3700000000000010 0.0000000000000000 0.0000000000000000  
 -7.1850000000000005 12.4447860000000006 0.0000000000000000  
 0.0000000000000000 0.0000000000000000 15.0000000000000000

C N Os

27 36 1

Direct

0.1178293090453230 0.0585782863169539 0.5184347516272756  
0.2718375641212076 0.0573478625244889 0.4840431169529177  
0.2719295079418027 0.2133704322978614 0.4933121087987654  
0.1156899211823066 0.3934285918096131 0.4792193529855546  
0.2672795481251721 0.3839641373759468 0.4965508696131806  
0.2721161763034197 0.5458872345204140 0.5200455472617850  
0.1173871673899194 0.7243795566369108 0.5009870041231248  
0.2744596918976834 0.7267146648805435 0.5226668214228941  
0.2745586241131908 0.8811901768916516 0.4873099169909844  
0.4510229153545962 0.0616138788891862 0.4864922877935945  
0.6067912005530612 0.0604564658917279 0.4972191926924386  
0.6058000112179032 0.2158901489176499 0.5227025508320182  
0.4460302763427967 0.3924419498763242 0.4974884157316068  
0.6082414581583471 0.3981449114870512 0.5240456033275802  
0.6076606616432717 0.5527681552975956 0.4952577934173363  
0.4524268976491772 0.7242676880047015 0.5226460659395219  
0.6165268586793118 0.7305821713839640 0.4834462110013410  
0.6074497440146054 0.8836465589350893 0.4925861703880869  
0.7832709901015759 0.0591692743936814 0.4948734037501812  
0.9401909741998693 0.0608463795719240 0.5173552404178366  
0.9396162211903315 0.2153594769627715 0.4810669238511311  
0.7838606992385534 0.3924183449371774 0.5221694116360123  
0.9374666911503432 0.3922312823909369 0.4825931106413042  
0.9396858942427291 0.5490758421918549 0.5003956307428108  
0.7889882448624794 0.7302321782588500 0.4756457942127680  
0.9424336668239179 0.7269825923842944 0.4984443409598710  
0.9413142622775713 0.8825813725124469 0.5167914866421605  
-0.0000708595953922 0.0010932224122402 0.5228314242785275  
0.1722003157869333 0.1654650834840694 0.5276300483302151  
0.1677883805153431 0.0019981093061934 0.5056669808630746  
0.3230295081070693 0.1626566407274088 0.4631585052861907

0.9976340565450961 0.3338529654685578 0.4764320436737102  
0.1697860329989981 0.4989280292050861 0.4959898136232767  
0.1697535355725638 0.3405763565347302 0.4628872327584048  
0.3191296388648435 0.4843385274022380 0.5410253031237627  
0.0003006353831868 0.6669549378434261 0.5003268310400528  
0.1688240093466988 0.8255789719177062 0.4686905886212830  
0.1676071690885106 0.6730491528401957 0.5333609548071301  
0.3304829683108308 0.8325424581788564 0.5093100934341162  
0.3323548988660108 -0.0003704424184868 0.4823246497557850  
0.4987759708464969 0.1654421858038959 0.5101176731172913  
0.5055159174136168 0.0108927051863379 0.4656578181508885  
0.6581555671774971 0.1600043625024269 0.5314839188776924  
0.3276276088258925 0.3290033629960011 0.4897643678291078  
0.5029396141159190 0.4909910080184602 0.4449333515907712  
0.4977223721542500 0.3517158099634226 0.5465620738701353  
0.6648630235269692 0.4971443805755229 0.4996191276376210  
0.3349891526760858 0.6647367729815843 0.5262674532594853  
0.5053440490592440 0.8308015275636846 0.5206428471950688  
0.5130839834565540 0.6728779880938359 0.5230922340734665  
0.6584411164682498 0.8330640563230631 0.4603186952048778  
0.6653019426185116 0.0004342359297243 0.4940336096260348  
0.8337832134358953 0.1600473137863894 0.4623446432734280  
0.8326329456664768 0.0079687620964190 0.5282395392955602  
0.9956270348907397 0.1669885547553802 0.5031241486914172  
0.6648666492507551 0.3332788056326771 0.5286011413988116  
0.8398076363711409 0.4999315813932501 0.5346766458094100  
0.8335088164242397 0.3365096393978848 0.5048445828181464  
0.9891903835888122 0.4984183071994730 0.4659974669250626  
0.6727486360856835 0.6729687672916842 0.4721008357815831  
0.8380969735491663 0.8351816827378664 0.4949098520431994  
0.8436202419101508 0.6777226343231493 0.4617646203776921  
0.9919371486775236 0.8266588541530451 0.5335742726304756

0.4766352290071932 0.5297691634217512 0.5679415669707697

**Pd doped g-C<sub>3</sub>N<sub>4</sub>**

C N Pd

1.0000000000000000

14.3700000000000010 0.0000000000000000 0.0000000000000000

-7.1850000000000005 12.4447860000000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 15.0000000000000000

C N Pd

27 36 1

Direct

0.1184021383791214 0.0597026638481871 0.5185924966912615

0.2732760757499567 0.0599671364765791 0.4836381334025202

0.2738231394120609 0.2164431933352007 0.5003432656425625

0.1177762145334364 0.3942204171357837 0.4785761878029417

0.2709218674098085 0.3893303318502321 0.4998989196275733

0.2717504203377260 0.5481956186854545 0.5191613384127602

0.1173358880381150 0.7259787055172547 0.4998671964003582

0.2741539207514020 0.7275845211656977 0.5189748965526307

0.2743165072707004 0.8821247876960241 0.4831585578823259

0.4523205470469702 0.0613588000029707 0.4824615176342004

0.6077278123144456 0.0595863589603228 0.4968457995279912

0.6070912045522129 0.2150874462571329 0.5192191588889488

0.4510800901923875 0.3981257170135376 0.5124445087432763

0.6078272507350355 0.3943191210232845 0.5185364708713245

0.6097451531788822 0.5481795342023330 0.4767790318768539

0.4528653989042264 0.7264765487683378 0.5175695802150783

0.6075382912896208 0.7261193129797380 0.4791235191015879

0.6078965267285953 0.8830773615317847 0.4953692783564071

0.7839650739617010 0.0592747516552522 0.4954252216420533

0.9406736604876830 0.0609797699463508 0.5172901675234802

0.9406664203833418 0.2150697312859779 0.4792869708437760

0.7851990045077462 0.3924445924276274 0.5192584605811705

0.9393609265964465 0.3933490360572500 0.4803589149556459  
0.9404882971147440 0.5497019884792292 0.4994297158313978  
0.7862758988157721 0.7281116002769270 0.4784938356240673  
0.9413298588734554 0.7265648723929004 0.4992862301648007  
0.9394908607189638 0.8817533387641076 0.5179228425330020  
0.9994278218754035 0.0008292809505713 0.5229067092444823  
0.1726372573463727 0.1661936379500222 0.5326880382508419  
0.1679876812029032 0.0037506584514651 0.5014805108829369  
0.3254376540795732 0.1667340989189899 0.4687918598557920  
-0.0003006413239751 0.3344812366590151 0.4742887468070098  
0.1680729897200119 0.4996049287013948 0.4967288632940337  
0.1729229996562111 0.3425811121615676 0.4628722307512812  
0.3189550890703030 0.4890244676611791 0.5385503534012622  
-0.0001245707117438 0.6675073120415648 0.4998141124308079  
0.1679071047710855 0.8269287294967217 0.4671834123388412  
0.1674199569379650 0.6751935716741184 0.5326992353145064  
0.3302839434575857 0.8329528400970441 0.5022380072745189  
0.3331001711155405 0.0009289477738027 0.4787796641547155  
0.5010414335951617 0.1655519779865898 0.5039237086480578  
0.5069353476128564 0.0100554154961252 0.4639113375623811  
0.6588049173939124 0.1594234122615086 0.5311534682973049  
0.3306244993371908 0.3329520329830979 0.5005052794507520  
0.5024283935118998 0.4953141210791427 0.4660130262520095  
0.5037434651329092 0.3467123216743136 0.5431784078435224  
0.6642460145054763 0.4960750251055324 0.4905562474261065  
0.3333191554906967 0.6669164707801459 0.5232347940260870  
0.5074367983307047 0.8334258254366793 0.5289723984237347  
0.5028190488762185 0.6701687812808150 0.5022688997953685  
0.6574915505383848 0.8321064569250147 0.4615502530794842  
0.6665080781637464 0.0004886028406086 0.4951717716708547  
0.8346519033498347 0.1599333242304222 0.4618427831287447  
0.8335876701795342 0.0088441320239389 0.5296310726836962

0.9965710956092984 0.1667365075282754 0.5007513387106827  
0.6669083343865230 0.3333244564313167 0.5240125863072552  
0.8405258432772256 0.4995505040319827 0.5337562858084193  
0.8352420039413122 0.3370098507930131 0.5012925367060170  
0.9904629072909233 0.4997244073888258 0.4644597257028917  
0.6682300004889041 0.6680974477745161 0.4720725753939721  
0.8348330074661825 0.8329532584743234 0.4983179622398018  
0.8416398801790200 0.6766287274675215 0.4642551350523479  
0.9910945058738673 0.8267828615569590 0.5333764631036813  
0.4597289347946447 0.5041720887471601 0.6134940611534079

**Pt doped g-C<sub>3</sub>N<sub>4</sub>**

C N Pt

1.0000000000000000  
14.3700000000000010 0.0000000000000000 0.0000000000000000  
-7.1850000000000005 12.4447860000000006 0.0000000000000000  
0.0000000000000000 0.0000000000000000 15.0000000000000000

C N Pt

27 36 1

Direct

0.1177316314910198 0.0589714995516923 0.5182459798211434  
0.2721016539152407 0.0578615428043782 0.4852287833110356  
0.2720439516214306 0.2140145303807554 0.4924880079914981  
0.1164128993579095 0.3942729782943003 0.4767473045933523  
0.2670868910666483 0.3842386487312530 0.4976849161795845  
0.2706123122691995 0.5466274360325867 0.5205623212472901  
0.1168891583728109 0.7245099376614909 0.5005636655906097  
0.2739553460168913 0.7277300631293004 0.5257933239360553  
0.2736929840625996 0.8817848677609627 0.4906792168877260  
0.4508045646722171 0.0603017935106127 0.4861060239821228  
0.6069148957886585 0.0603324168385378 0.4851788445426363  
0.6068685698383161 0.2137115713260060 0.5212352789176210



0.4489324777820093 0.3921293448030105 0.5057879800766115  
0.6063266822416747 0.3927100565159187 0.5255621449408695  
0.6082975287105488 0.5499767645656359 0.4981894096886136  
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0.6162067334980367 0.7331179228767858 0.4917959643033472  
0.6075012786186442 0.8851191829478532 0.4797079359971058  
0.7841653030314117 0.0598939675346915 0.4836579853175631  
0.9397582303046622 0.0607861260665035 0.5151275293327149  
0.9411461383199635 0.2160168685440834 0.4782897883544676  
0.7847029269368502 0.3906746359016268 0.5230847999384891  
0.9388694136545284 0.3929880241645923 0.4825842886686087  
0.9394559560006447 0.5486306972343624 0.4994049717239317  
0.7870436858075279 0.7282100276288622 0.4860753200962279  
0.9417542885428291 0.7263683339902117 0.5000021954796453  
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0.9991432780684770 0.0009448688393393 0.5231318045181804  
0.1715302106759461 0.1659638004835917 0.5254422396237464  
0.1681393969339231 0.0026633162766535 0.5077143751442891  
0.3231008728210090 0.1626971923022449 0.4629912263524276  
-0.0003166641768931 0.3350083332255746 0.4745182239746083  
0.1698577386922947 0.5007689930308171 0.4921643243793560  
0.1703667898820913 0.3413793366809076 0.4608868956122695  
0.3122747477852357 0.4824469300807996 0.5432776976055247  
-0.0003807639924223 0.6665956450154126 0.5002122109015803  
0.1689416608175678 0.8256026646066396 0.4681674888622640  
0.1667126937365861 0.6728000954211972 0.5322211085199898  
0.3291894378021428 0.8346475381861989 0.5183392121250445  
0.3319141339008521 -0.0004361979448094 0.4839775899556991  
0.4987067027768011 0.1605359392792017 0.5179068155413546  
0.5044980046141088 0.0118359877627697 0.4560064912161910  
0.6604488412854540 0.1589337390917406 0.5201183693646588  
0.3284237743501265 0.3298612991245071 0.4915620674044486

0.5058778004929919 0.4915035714097233 0.4536420368347701  
0.4993134428171497 0.3371521826932566 0.5307600155141710  
0.6642516579168526 0.4993111082802755 0.5178770502436357  
0.3349232590371055 0.6667538802018415 0.5284056411860489  
0.5027871677343101 0.8333261204373129 0.5003138473769686  
0.5192176185783361 0.6872375063978315 0.5388446298635265  
0.6584461618574550 0.8308989787772808 0.4567866183982928  
0.6659355589010235 0.0010764830229255 0.4793469655362214  
0.8371855198577771 0.1618636255460928 0.4532671909925305  
0.8315381929060630 0.0074213599171969 0.5178119237550010  
0.9954182914623246 0.1682264377612491 0.5066594709421677  
0.6668179428415744 0.3313363772037952 0.5283360850757864  
0.8399245158596443 0.4985402535303393 0.5337268858078920  
0.8367805815629235 0.3360504078178357 0.5087848388831085  
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0.6706847510392967 0.6713097320800941 0.4834904201833208  
0.8349434506216988 0.8319358083644148 0.5090425499572527  
0.8411237822757104 0.6765645990599167 0.4666787350314079  
0.9933302182921825 0.8272433310960047 0.5322548361112630  
0.4710353515971163 0.5308873300649248 0.5728337350132975

### Re doped g-C<sub>3</sub>N<sub>4</sub>

C N Re

1.0000000000000000  
14.3700000000000010 0.0000000000000000 0.0000000000000000  
-7.1850000000000005 12.4447860000000006 0.0000000000000000  
0.0000000000000000 0.0000000000000000 15.0000000000000000

C N Re

27 36 1

Direct

0.1175200890150172 0.0581207584285412 0.5176653026356088  
0.2716045408866046 0.0568137277680615 0.4835074109504230

0.2714928068275013 0.2126601580391279 0.4910824058544460  
0.1170094242563537 0.3935855143525732 0.4810816537344080  
0.2691744023464106 0.3838457410703092 0.4924302018592523  
0.2751700706238484 0.5472635015478271 0.5189016226246790  
0.1172580184906825 0.7244339624859362 0.5007130355367839  
0.2743068992785122 0.7265826949683326 0.5221974224319793  
0.2743797808840140 0.8810211612072767 0.4867797753462605  
0.4509885628269943 0.0613806391002571 0.4862251084102481  
0.6070696778957954 0.0609137848007178 0.4964133476046926  
0.6053894510851234 0.2159371205543008 0.5223429686007104  
0.4451997358682118 0.3929858852737781 0.4982612884593791  
0.6064856093263314 0.3976194962455469 0.5238288567877931  
0.6047802441694484 0.5521271859964204 0.4922025076957626  
0.4533511521739562 0.7252453115268229 0.5235211812190137  
0.6157563992579438 0.7308954742187029 0.4846442305966021  
0.6077228735901482 0.8843689366860148 0.4928111242860578  
0.7835538080908794 0.0597173631355857 0.4950266776604950  
0.9401774115062020 0.0607419471823944 0.5180805333293260  
0.9402895106829029 0.2157373431966199 0.4829277697352869  
0.7836704741553815 0.3925627770100950 0.5221050189156020  
0.9382464189856777 0.3927114978944106 0.4846865613312985  
0.9397218578556431 0.5492902619428640 0.5005828253421359  
0.7879784910019209 0.7294565083139658 0.4763592620997129  
0.9418210743296235 0.7266512809423152 0.4985645544797975  
0.9405890249692959 0.8820432523326539 0.5171186683067882  
0.9995260597094416 0.0006359487604457 0.5228424864922631  
0.1717365231414661 0.1651166876844722 0.5253730812195353  
0.1677058632400647 0.0015976519874658 0.5058250953278437  
0.3227504692403670 0.1618115314045847 0.4617194069632701  
0.9989969092621137 0.3345936876414790 0.4789047728481060  
0.1713474074836961 0.4988720931848077 0.5004552868627891  
0.1702046177889509 0.3406952398686935 0.4613510077299891

0.3246593877972570 0.4858039405898184 0.5345006469342362  
0.0000703956812834 0.6669106498967086 0.5002315955682848  
0.1685300036633169 0.8254613211479787 0.4682591021124461  
0.1674934165498014 0.6730596836463731 0.5331250526406972  
0.3302583012383872 0.8322968027619166 0.5085424211731495  
0.3321626504421425 -0.0008006702450723 0.4820047693686791  
0.4982208877388195 0.1648709318714685 0.5106212455195147  
0.5057084130000987 0.0110851442336834 0.4648256233717249  
0.6582043507819445 0.1605435643243465 0.5304724682281491  
0.3273633332672997 0.3280501991492222 0.4870380534196276  
0.5000340052997008 0.4909541985933744 0.4456420809234720  
0.4973252934873125 0.3508841854671613 0.5466417726237415  
0.6623706598713065 0.4970457452920508 0.4983721572164075  
0.3357793493654255 0.6651666907226926 0.5259849541626413  
0.5055466795171358 0.8316106657469794 0.5204759335774751  
0.5135459190628336 0.6733971207045600 0.5264779268899613  
0.6579687013185732 0.8329668603153354 0.4606232148254386  
0.6657530782177653 0.0012301212550997 0.4938185546310599  
0.8347868027220856 0.1610138561854914 0.4631311077951963  
0.8325428126258412 0.0078307764700935 0.5277069032619079  
0.9958903608965300 0.1673008183934402 0.5058351370657250  
0.6645048524584979 0.3336188062640624 0.5279637529310744  
0.8391872042621433 0.5001977467596425 0.5334977227319665  
0.8341982085317047 0.3368793685188800 0.5067019173199185  
0.9900311663928747 0.4987004596750805 0.4676316065020659  
0.6713977715496238 0.6726268577870672 0.4721754350186694  
0.8371749359365467 0.8344176061322597 0.4957621490127028  
0.8427507975077588 0.6771157732657308 0.4623033295500844  
0.9914748342097672 0.8263450698411064 0.5335562246029839  
0.4779904611679214 0.5281656690508109 0.5735807675402683

**Rh doped g-C<sub>3</sub>N<sub>4</sub>**

C N Rh

1.000000000000000

14.3700000000000010 0.000000000000000 0.000000000000000

-7.1850000000000005 12.4447860000000006 0.000000000000000

0.000000000000000 0.000000000000000 15.000000000000000

C N Rh

27 36 1

Direct

0.1177544406441246 0.0583676098606044 0.5185172655837458

0.2721149354962865 0.0577480738031092 0.4842722852080106

0.2720774381842070 0.2138550573145533 0.4942007955536049

0.1166199678507249 0.3938767249547053 0.4781048538902046

0.2685431234639681 0.3856388857611951 0.4982320621959233

0.2715533533274035 0.5466252706982626 0.5196723543794068

0.1168542899525424 0.7247876103170335 0.5007257622827702

0.2738877233932153 0.7272410804769838 0.5229096118041457

0.2740819095414046 0.8815863541196429 0.4872407785209023

0.4515922141320390 0.0609260444780146 0.4863394798836084

0.6074508846635583 0.0603174137384101 0.4959626641548424

0.6068099666790481 0.2151287563245741 0.5228486480719038

0.4486690133546831 0.3914252261662944 0.4989852780399261

0.6077866140199204 0.3950587585592040 0.5224675038932624

0.6056968261093513 0.5503951748317359 0.4938988382672056

0.4533223823052424 0.7272456338612624 0.5225357411786993

0.6142802188433261 0.7309870080336206 0.4838031724894561

0.6080166282467498 0.8849086199022882 0.4907739392146315

0.7840976319601336 0.0597737290357665 0.4939618087475088

0.9405101900426304 0.0606904098138285 0.5171789866177517

0.9407081680697817 0.2154620485409773 0.4806637552145480

0.7848164690603311 0.3916190884415836 0.5223223363637238

0.9387546751436912 0.3927340129953619 0.4826700267230296

0.9399148839688594 0.5489362776571650 0.4998711678025274

0.7868243695971848 0.7287206828370465 0.4774903223640599  
0.9409336701826034 0.7259771398376822 0.4982265499044315  
0.9400116649008589 0.8817612245953838 0.5166112665115897  
0.9994215222862326 0.0005741509746029 0.5224230295645503  
0.1719509611462724 0.1653108888623118 0.5279887825570693  
0.1680098294680190 0.0021210318743466 0.5062010800499411  
0.3229597094890731 0.1629300747061686 0.4634264237410180  
0.9992754231379383 0.3344286790279785 0.4759112221834916  
0.1699932774514781 0.5002838134608798 0.4930816607576896  
0.1708713603229423 0.3411658559031156 0.4632086569196464  
0.3164628893904941 0.4850679197847351 0.5416737283038503  
-0.0003939262540701 0.6666967390241809 0.4997400596572538  
0.1683429769547971 0.8259157944766012 0.4683368875956644  
0.1669036560262363 0.6735099318194642 0.5334260191843602  
0.3299410013312041 0.8330972079583865 0.5096413338835024  
0.3324734759348099 -0.0002950388020250 0.4821952408131547  
0.4995296757407877 0.1637210118931433 0.5119802134866365  
0.5063690768803041 0.0110083881491885 0.4635759921075834  
0.6591447052212612 0.1593454366632728 0.5309157670490968  
0.3288801375844119 0.3300698375160599 0.4927243350356167  
0.5024464170880845 0.4906603794664482 0.4506674738322159  
0.4990218639838171 0.3411304398359246 0.5327233300447758  
0.6637385126703296 0.4996749716497885 0.5102517367854114  
0.3345797036285897 0.6661261382196895 0.5267755626760013  
0.5059310040997155 0.8337796298513713 0.5199628649426322  
0.5132109939380229 0.6772247681149909 0.5228868761867753  
0.6575932567669149 0.8332965943108713 0.4578429679668284  
0.6662794859989114 0.0011395264830331 0.4925814443324091  
0.8350995954095515 0.1606908437536383 0.4614604543127637  
0.8328966686333302 0.0082478180523824 0.5275974479791625  
0.9963145531123683 0.1670834988528655 0.5033726173876891  
0.6667596073851537 0.3328750690813183 0.5275830535748542

0.8402425432798899 0.4992331159621303 0.5343726914271525  
0.8355365385571427 0.3362621263684947 0.5060926977561029  
0.9897146814645924 0.4986576126914734 0.4651982263006967  
0.6701956450432174 0.6715858521705692 0.4746818134409361  
0.8361723274670336 0.8339249847385241 0.4962263419253957  
0.8412899176576657 0.6760653337804456 0.4629228658946320  
0.9909091590283274 0.8260873428357286 0.5323931106893455  
0.4741488143495040 0.5322944041023748 0.5715048145902835

### **Ru doped g-C<sub>3</sub>N<sub>4</sub>**

C N Ru

1.000000000000000  
14.370000000000010 0.000000000000000 0.000000000000000  
-7.185000000000005 12.444786000000006 0.000000000000000  
0.000000000000000 0.000000000000000 15.000000000000000

C N Ru

27 36 1

Direct

0.1181285106920803 0.0591117812847063 0.5186832574997531  
0.2723740765877518 0.0582240973031013 0.4846443754912402  
0.2725164146402094 0.2143882167776665 0.4941595027342146  
0.1159560844439073 0.3935182360078606 0.4786069529719214  
0.2681283773225038 0.3855739558210908 0.4973384434219092  
0.2714027793292342 0.5461788880813220 0.5197509120786821  
0.1171553246825435 0.7246187624957001 0.5002385401568898  
0.2741496661846236 0.7270885990871251 0.5230211738068093  
0.2743130417719979 0.8815823887401837 0.4877019191421690  
0.4511829605267769 0.0612990990424165 0.4871342846422755  
0.6068710559796600 0.0599615878364985 0.4969901865698030  
0.6063669857035368 0.2155264223593898 0.5228907893848046  
0.4479829432519735 0.3928572441855932 0.4970667925537257  
0.6085993595936620 0.3973348328215210 0.5240035875701857

0.6067578103716088 0.5522461610050170 0.4955174230666455  
0.4519128386349728 0.7239260796766631 0.5216033151995266  
0.6150447427696546 0.7295742009835816 0.4825905039057721  
0.6073034298056228 0.8832121071686145 0.4921876026556761  
0.7833970602949898 0.0589641376225084 0.4947917137903651  
0.9403053012699466 0.0606347420814479 0.5174204588414122  
0.9398641720882328 0.2150994322095144 0.4808081432544619  
0.7844759811511083 0.3920670926874862 0.5226244079684188  
0.9379383524856908 0.3921477193105209 0.4825919457916497  
0.9398704603580288 0.5488883167611964 0.4995271658933890  
0.7882007940395914 0.7297322940121030 0.4757706920903179  
0.9417541591336117 0.7263841912652241 0.4975539224578267  
0.9410920586832232 0.8822455956755180 0.5160683757412513  
-0.0000288128344389 0.0010344402231879 0.5225863241122701  
0.1724310327304203 0.1661350020584170 0.5279090439015626  
0.1683744828913161 0.0027633652359501 0.5065315678359759  
0.3234335094150882 0.1634909242159660 0.4637213059935022  
-0.0018600592692558 0.3337837619755528 0.4758914606149822  
0.1693194848210380 0.4992817526116302 0.4948553758297252  
0.1706088187045960 0.3411234185395219 0.4629955610018790  
0.3181293715403349 0.4853268379945916 0.5412453807881927  
0.0000322666848904 0.6667345037669314 0.4991550763928525  
0.1687804523551217 0.8259866445698957 0.4681563435787854  
0.1671442161228180 0.6732380834588597 0.5327984667131460  
0.3301190807280906 0.8331310640343367 0.5105960178016123  
0.3325455212176292 0.0000525050692747 0.4827643855019811  
0.4992008056300298 0.1648553206000756 0.5113899925595102  
0.5054517625924230 0.0104629147181212 0.4657061683792186  
0.6587950994964126 0.1597215605423722 0.5307768162471118  
0.3289130924107389 0.3305882959731157 0.4914562132764915  
0.5034429008732892 0.4921852315861590 0.4483495080583565  
0.4975767563359502 0.3475489848681630 0.5408249770075138



0.6649063360485745 0.4988232150125320 0.5056631457705548  
0.3343222657068564 0.6649998340728580 0.5263223060046737  
0.5051063682831782 0.8305332050080808 0.5206937228459680  
0.5115589158986058 0.6719488217626997 0.5198512010044448  
0.6580060907983493 0.8326160595234128 0.4598988475164154  
0.6652728062428902 0.0000194372534055 0.4938730743655666  
0.8340228609435648 0.1597932627373502 0.4620044876662451  
0.8327359142068401 0.0079079340424039 0.5284420851011188  
0.9957911052820990 0.1667957132618365 0.5030158038246468  
0.6657909564762230 0.3332027108600793 0.5284357597147591  
0.8402538169187418 0.4996975113046663 0.5342947632925462  
0.8345884525556109 0.3363086291130822 0.5063320312680553  
0.9891021545982422 0.4981248214934629 0.4647860307844415  
0.6719214387093809 0.6722827336352382 0.4730701730260414  
0.8376880479508002 0.8348999658608579 0.4945797928198065  
0.8426014779268645 0.6769312686076846 0.4615078453083787  
-0.0083607996533064 0.8262390790056112 0.5323601888844918  
0.4751379616714411 0.5318310936698072 0.5699084463237167