

## Supplementary Information

### Tunable formaldehyde sensing properties of palladium cluster decorated graphene

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## CONTCAR-(Pd1/Graphene)

1.0000000000000000

9.8734998702999999 0.0000000000000000 0.0000000000000000

-4.9367499351999999 8.5507017119000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.0000000000000000

C Pd

32 1

Direct

0.0832254772237793 0.1664361999688388 0.4986735785009399

0.1665501593756694 0.0832229601523812 0.4983322172703136

0.3332402248116622 0.1664663753073736 0.4979372627670946

0.4167126691225730 0.0833562371518780 0.4974846814550731

0.5832873238774301 0.1666437738481194 0.4974846814550731

0.6667598411883434 0.0835336356926238 0.4979372627670946

0.8334497976243309 0.1667770508476162 0.4983322172703136

0.9167744927762180 0.0835638110311585 0.4986735785009399

0.0831732208521191 0.4165867676246018 0.4993544181062873

0.1662434157554549 0.3328562191034269 0.4996332463022226

0.3323285953580581 0.4149124565210689 0.5011881506734637

0.4164722210208543 0.3327349498810220 0.4990740705826008

0.5835277917810580 0.4162629038194147 0.4990740768780449

0.6667597205753270 0.3332259351960187 0.4979372641164295

0.8334499212326900 0.4166730066464724 0.4983322270234079

0.9168204487204690 0.3334101281809815 0.4984696557015399

0.0832255248276202 0.6667894308402378 0.4986736032527742

0.1662433905508698 0.5833869823551884 0.4996332627574260

0.3323285668917408 0.6674162772607684 0.5011881561621718

0.4153375711360154 0.5826687319350372 0.5042769826923357

0.5846624308639849 0.6673312960649651 0.5042769826923357

0.6676714841082597 0.5825837507392340 0.5011881561621718

0.8337565504491290 0.6666130456448139 0.4996332627574260

0.9167745021723712 0.5832105971597645 0.4986736032527742

0.0831795952795276 0.9165899838190208 0.4984696557015399

0.1665500807673105 0.8333270213535301 0.4983322270234079

0.3332403714246737 0.9167741768039834 0.4979372641164295

0.4164722342189441 0.8337371241805879 0.4990740768780449

0.5835278229791421 0.9172651621189875 0.4990740705826008

0.6676714786419408 0.8350875714789336 0.5011881506734637

0.8337565922445388 0.9171438928965753 0.4996332463022226

0.9168268051478830 0.8334132603754003 0.4993544181062873

0.5000000009999965 0.6250000140000012 0.5726543045157406

## CONTCAR-(Pd2/Graphene)

1.0000000000000000

9.8734998702999999 0.0000000000000000 0.0000000000000000

-4.9367499351999999 8.5507017119000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.0000000000000000

C Pd

32 2

Direct

0.0830857197579603 0.1658414504203972 0.4994922264238991

0.1665347552002468 0.0827234618341339 0.4988955579015019

0.3332294958374913 0.1658469499462513 0.4989909318537652

0.4166897814219594 0.0828042646399509 0.4980611315639590

0.5831958986187636 0.1664328281324920 0.4980674947094841

0.6666504821359781 0.0833881005121597 0.4990084686145465

0.8333504253060837 0.1664673701390445 0.4989104657952770

0.9168285488029286 0.0833860927653158 0.4995016758931296

0.0827120398788069 0.4161794826361134 0.4990718189126364

0.1648978606209052 0.3317460949553318 0.5010581150544916

0.3319918419367009 0.4137459878924296 0.5047580023792821

0.4169071883044698 0.3315585284138992 0.5011064429204888

0.5835660080133389 0.4160015213571242 0.4999221456431180

0.6667922655727472 0.3328887383400533 0.4979634967810511

0.8332589841483543 0.4163054244091985 0.4974876236194709

0.9165974674602110 0.3329916004890822 0.4980326550735122

0.0832313569936680 0.6663844296936822 0.4971961355382210

0.1662537371885894 0.5832188003340610 0.4987159199900730

0.3321498116946059 0.6673172774675387 0.5017851552714196

0.4147023566910450 0.5826291057868723 0.5077246944885506

0.5851406925881821 0.6666458385913063 0.5077178503183266

0.6676554334884620 0.5819211518304254 0.5017944542479933

0.8335622334595705 0.6659806842907283 0.4987508870493083

0.9166094573131629 0.5828491241809541 0.4972101961056782

0.0832678497047236 0.9161988008100291 0.4980296188096354

0.1666202355428756 0.8329091505504603 0.4974772239446172

0.3330899418778669 0.9163411968472054 0.4979515333542445

0.4163039016645114 0.8332331512874553 0.4999067609516455

0.5829574619343751 0.9176856690690430 0.5010959317948993

0.6678870841412765 0.8355216099661150 0.5047130873696448

0.8349864189325594 0.9174827788191124 0.5010554791000826

0.9171429939914798 0.8330138641812372 0.4990853165256008

0.3577081847901011 0.4936985568574787 0.5749801065916864

0.6424123969859928 0.7564516675533343 0.5749413844087484

## CONTCAR-(Pd3/Graphene)

1.0000000000000000

9.8734998702999999 0.0000000000000000 0.0000000000000000

-4.9367499351999999 8.5507017119000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.0000000000000000

C Pd

32 3

Direct

0.0836851986204081 0.1587056972992931 0.4971342216459326

0.1667422750396362 0.0753743162940109 0.4968640277401694

0.3333848550956070 0.1582775968169136 0.4974997479316346

0.4171130625924381 0.0753690107210894 0.4968600175985901

0.5835135432027811 0.1587035018625176 0.4971249411485135

0.6673004499163417 0.0760930757789671 0.4972818779409470

0.8337932592400268 0.1590693715085679 0.4968060825099070

0.9172901086931532 0.0760919575234600 0.4972796744831759

0.0833512045629775 0.4089696234669647 0.4969664129668509

0.1657410722978108 0.3247461229977372 0.4986859938083577

0.3320943550777523 0.4065536692314837 0.5034511860996935

0.4159698169446073 0.3233979163296807 0.5007846256530581

0.5830430133031861 0.4065664287883181 0.5034323680339901

0.6675461152419990 0.3247539700157906 0.4986532378776330

0.8341772194773517 0.4089885516133336 0.4969149538937811

0.9172032021260577 0.3258874622105359 0.4961122743677870

0.0838174664155482 0.6590402343687024 0.4958590428192652

0.1667461300037253 0.5756821200318866 0.4970812871318437

0.3324890194418824 0.6596492239710021 0.5008452070873659

0.4141441377929047 0.5749336237013258 0.5080807426827215

0.5851534848622667 0.6616146990170531 0.5107819974992830

0.6694498381624668 0.5749439868352652 0.5080339234098509

0.8357714528876838 0.6596876753752674 0.5007680381367665

0.9175074996937849 0.5757106164340657 0.4970213678595443

0.0837895759481446 0.9088690357712869 0.4966608850952687

0.1670571794261883 0.8255754616108752 0.4962336186384870

0.3336398266417576 0.9088622748229337 0.4966725101374176

0.4165359239344564 0.8256970767405039 0.4989423368121134

0.5835455220368145 0.9103665321233577 0.4997630872063720

0.6688852773823685 0.8291660615666636 0.5039197434738065

0.8353956568484859 0.9103789228060680 0.4997537077716800

0.9177171304134059 0.8257248061845854 0.4988991208157750

0.3581127408056144 0.4918860863399151 0.5761240388812812

0.6426231042858914 0.4914690511952364 0.5760494201367404

0.6366905725844548 0.7638048316453320 0.5759483427043889

## CONTCAR-(Pd4/Graphene)

1.0000000000000000

9.8734998702999999 0.0000000000000000 0.0000000000000000

-4.9367499351999999 8.5507017119000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.0000000000000000

C Pd

32 4

Direct

0.0890806342638598 0.1677742292144847 0.4981283043293541

0.1723953684590075 0.0846494056159512 0.4977118864174458

0.3390673054020298 0.1676937289455325 0.4981845785685587

0.4227218575542420 0.0846819501836854 0.4976992181475467

0.5891642328634533 0.1678181923258063 0.4981221917729425

0.6726787616012009 0.0850460665037499 0.4981690650374452

0.8393058315258284 0.1681286416774742 0.4978127670511532

0.9227824407357280 0.0849789568981483 0.4981893681795753

0.0888204550307413 0.4180169779751968 0.4968812127383118

0.1710557171867621 0.3339628332582769 0.4985972406390790

0.3380735165774315 0.4167487135759884 0.5012739126902120

0.4215406931404816 0.3327594715100913 0.4999974138062323

0.5890041862411460 0.4167448592988890 0.5013614444813383

0.6732925655760449 0.3339914953843419 0.4986447345294271

0.8395824426471835 0.4179881435070920 0.4969277078056312

0.9224995200451990 0.3345683310178265 0.4968093170151889

0.0893926818000475 0.6684215127611927 0.4955948415736151

0.1723080479582856 0.5849765273397137 0.4960996379693872

0.3383640682635510 0.6687838798696354 0.4974918772928997

0.4214476414546512 0.5850475870533880 0.5011640292636830

0.5898619929148042 0.6694452779806357 0.5014975202522438

0.6739031360347385 0.5850492151294273 0.5013182273372654

0.8407577445979514 0.6687166935316446 0.4976623598505699

0.9230119946207774 0.5849451564800737 0.4962001057503372

0.0895835125938345 0.9183708073456571 0.4968719762344579

0.1726827223117890 0.8349714659417670 0.4961706199620985

0.3392003069273315 0.9184139206495660 0.4968144442402632

0.4222391389479306 0.8352336810530830 0.4975549737713684

0.5887159888642247 0.9191923155012356 0.4989824092058694

0.6733313057362056 0.8363236573506485 0.5007469643347948

0.8408177747493611 0.9191185379991084 0.4990255336078877

0.9233578200836720 0.8351562179960804 0.4976735342485941

0.3715857411064863 0.4991516802537672 0.5752038190767734

0.6362466820147678 0.4989438585524340 0.5752857208026665

0.6408675098661440 0.7731047654700335 0.5760164983683045

0.5501189223031073 0.5920820388483760 0.6456044196474806

## CONTCAR-(Pd5/Graphene)

1.0000000000000000

9.8734998702999999 0.0000000000000000 0.0000000000000000

-4.9367499351999999 8.5507017119000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.0000000000000000

C Pd

32 5

Direct

0.0860128277595978 0.1636126968273202 0.5020376652122098

0.1701231804408085 0.0796901737186842 0.5004514466505271

0.3370961180689557 0.1645909527275405 0.4958035538934848

0.4191034681842803 0.0796672043261176 0.5004633933093897

0.5871866956033485 0.1636450393884173 0.5020296964596734

0.6702586804960998 0.0792572803473179 0.5017550429684093

0.8363158365270302 0.1630882353121721 0.5011482487199914

0.9185485046076611 0.0792667807629941 0.5017646564614049

0.0858314524708352 0.4136954706509196 0.4980055805623855

0.1686687070351937 0.3305129254933951 0.4988253750627957

0.3363713864410014 0.4127949515742066 0.4979279224403482

0.4195172229372507 0.3294671658598792 0.4927959505835459

0.5859972719494703 0.4128244952896622 0.4979443168870508

0.6714371927839642 0.3305475826013329 0.4987805607603958

0.8374457298482624 0.4137362499715073 0.4979848957905078

0.9198350830584379 0.3301142892200717 0.4990120713834378

0.0863938129904059 0.6632201069678081 0.4970427789981094

0.1694397933423025 0.5802369272639211 0.4973541085309812

0.3358547262927819 0.6642059662815510 0.4992092333856615

0.4200801309125975 0.5814166302787193 0.5006469222698985

0.5873389320792045 0.6651435941634418 0.5004259308262946

0.6708798692024652 0.5814331851868221 0.5006821110796004

0.8379125122667676 0.6642251872761077 0.4992271751932907

0.9203612892001646 0.5802695708511734 0.4973508379100280

0.0860929756338835 0.9121146048723332 0.4994353212133745

0.1694618299624532 0.8294178118166121 0.4981336298222238

0.3355061029801701 0.9120966083958634 0.4994451343621178

0.4193634059623721 0.8301093385345634 0.5000398903102555

0.5865160684641720 0.9135109768132800 0.5011251788684580

0.6700558504870504 0.8306071202683020 0.5008447845345396

0.8364996950089046 0.9135197754535493 0.5011246868946136

0.9202486196459388 0.8301277936332404 0.5000371955770255

0.3524235048006885 0.4579327682384036 0.5717785899157890

0.6138050752365840 0.4588431369275232 0.5718295012321286

0.1872313698526565 0.1450698130670750 0.5725409006708286

0.4673944284364472 0.1458905193057039 0.5725473702327845

0.4045409930297860 0.3007580433324616 0.6342786960264488

## CONTCAR-(Pd6/Graphene)

1.0000000000000000

9.8734998702999999 0.0000000000000000 0.0000000000000000

-4.9367499351999999 8.5507017119000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.0000000000000000

C Pd

32 6

Direct

0.0886336740457583 0.1669323462888780 0.4959940106370775

0.1706656023937377 0.0823543324458343 0.4967948026831999

0.3376294876442483 0.1641452624934155 0.5000990349597596

0.4228418717035260 0.0823936392086601 0.4967786873789639

0.5894589044982005 0.1669590564543761 0.4959962679585672

0.6726245913684658 0.0842369320991447 0.4947363602990781

0.8392346644527728 0.1672766211262427 0.4939762924100345

0.9227707221215178 0.0841929457203373 0.4947456380300159

0.0887431310666997 0.4168856361853474 0.4948014579898746

0.1708852689621494 0.3332391686501676 0.4980130912115788

0.3362685268641121 0.4164640636387417 0.5053471178039601

0.4212281510170036 0.3313057971021936 0.5067633635438785

0.5913167600189109 0.4164550450297296 0.5054141145445793

0.6735123436082772 0.3332777691440625 0.4980510362964336

0.8393224984978148 0.4168950779083233 0.4948522768184637

0.9223677426840545 0.3335466438009007 0.4934537659642930

0.0890967376078400 0.6669811492424288 0.4933779548945020

0.1721540895463477 0.5836706983094965 0.4947637303677671

0.3379546714639914 0.6673193346408057 0.4980138997728526

0.4200588285071704 0.5840790774985444 0.5053631905883843

0.5901462357579790 0.6692053244494847 0.5069907745704346

0.6751452176900973 0.5840924620575149 0.5055250419669520

0.8405142848832191 0.6673023207138837 0.4981717026713781

0.9227002128652582 0.5836823344957366 0.4948627445238725

0.0886510399607691 0.9163041599532371 0.4945994736029555

0.1722563889249217 0.8332790762356463 0.4937680065281023

0.3388752277384031 0.9163495482155800 0.4945383062606409

0.4220346780024499 0.8336438761064521 0.4960085991960585

0.5886369365624951 0.9182141008011084 0.4970259175483914

0.6738174823089289 0.8364676920475814 0.5005170494434116

0.8407441942260251 0.9181786104726050 0.4970663067432918

0.9227724606305328 0.8336103444397757 0.4961189367819814

0.3690895869634609 0.4982877367241407 0.5813564034416369

0.6384050555990006 0.4994828381030779 0.5815700041706322

0.6424249193704685 0.7775507795652564 0.5716377246733121

0.5751254726526686 0.6453973616593572 0.6502244076043696

0.3652097253576617 0.2204179273269059 0.5711840133640561

0.4295435184330537 0.3499246006450282 0.6499884377552609