

Supporting Information (SI)

Cluster Formation Effect of Water on Pristine and Defective MoS₂ Monolayers

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Figure S1. Electronic band structures by vdW-DF-cx and G₀W₀ for pristine and defective MoS₂ monolayer.

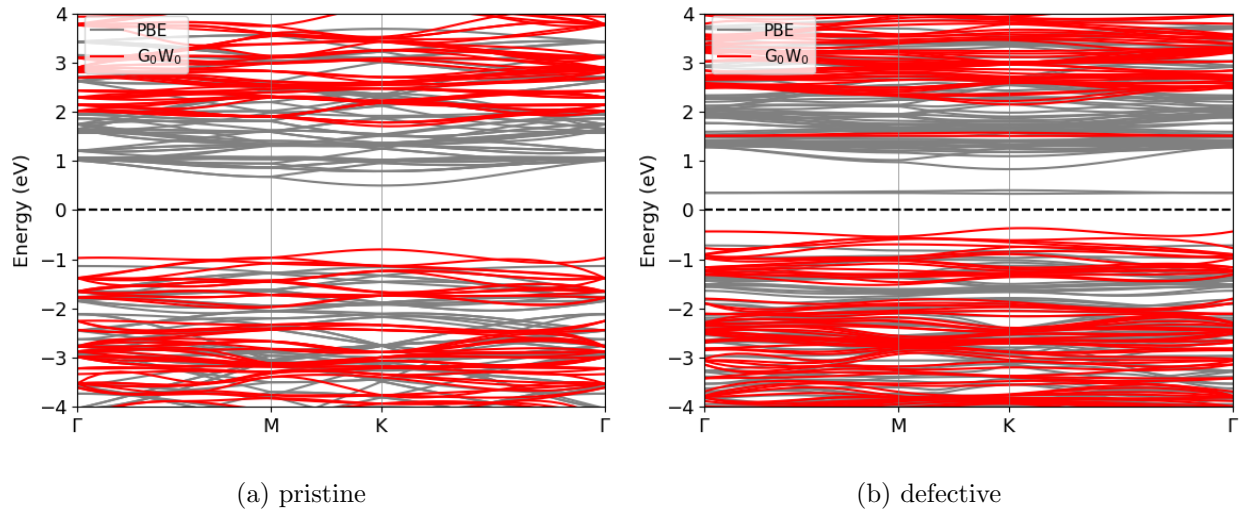
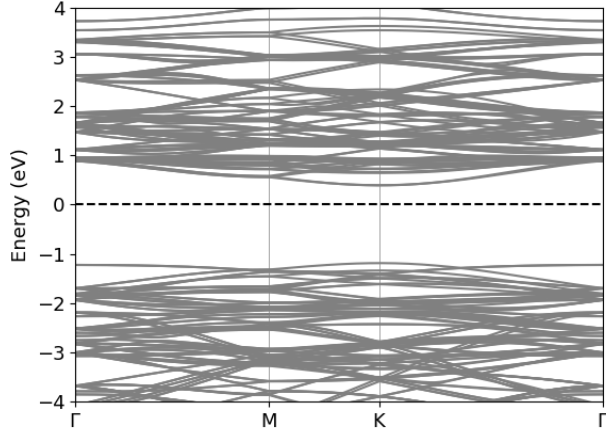
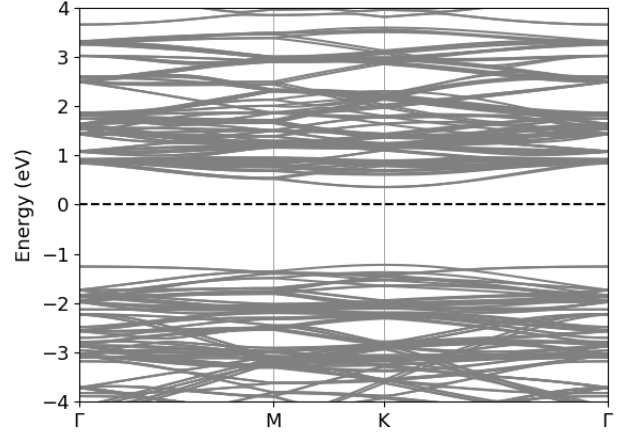


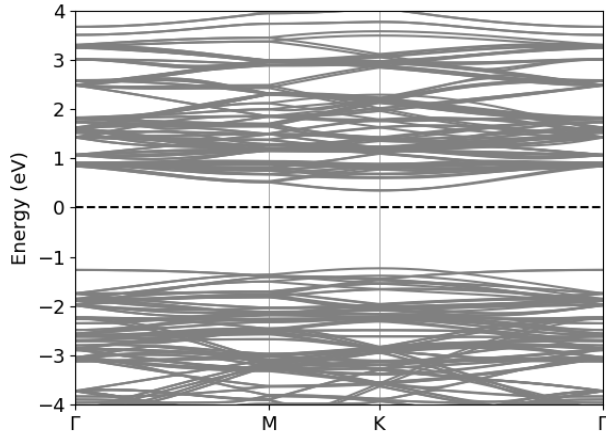
Figure S2. Electronic band structures for $(\text{H}_2\text{O})_n$ ($n=1-5$) on pristine MoS₂ monolayer by vdW-DF-cx functional.



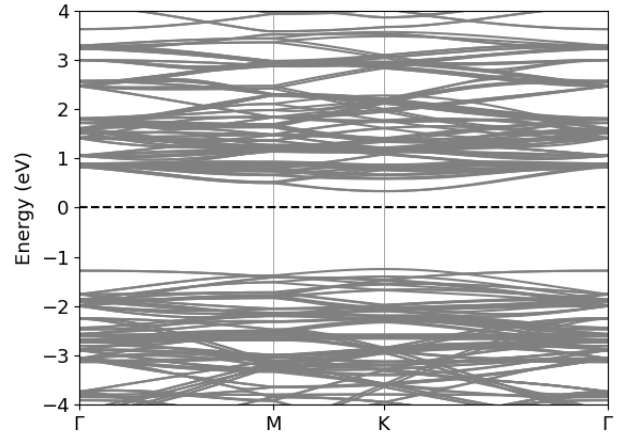
(a) $(\text{H}_2\text{O})_1$



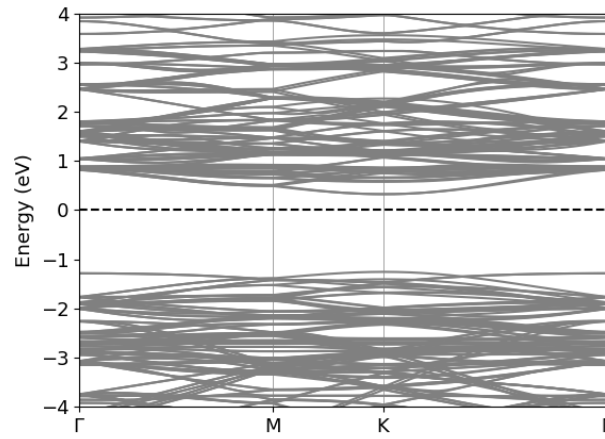
(b) $(\text{H}_2\text{O})_2$



(c) $(\text{H}_2\text{O})_3$



(d) $(\text{H}_2\text{O})_4$



(e) $(\text{H}_2\text{O})_5$

Figure S3. Electronic band structures for $(\text{H}_2\text{O})_n$ ($n=1-5$) on defective MoS_2 monolayer by vdW-DF-cx functional.

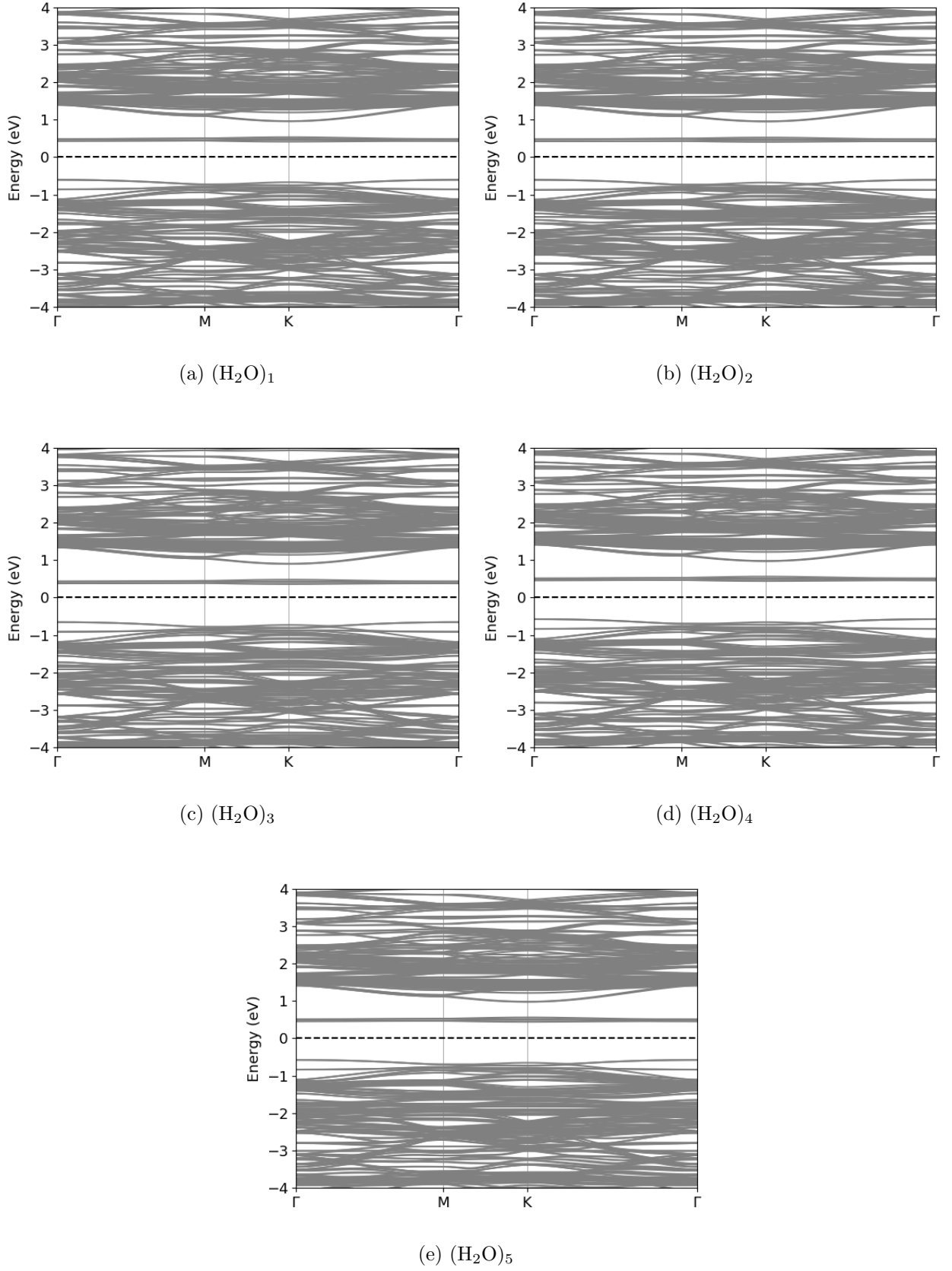
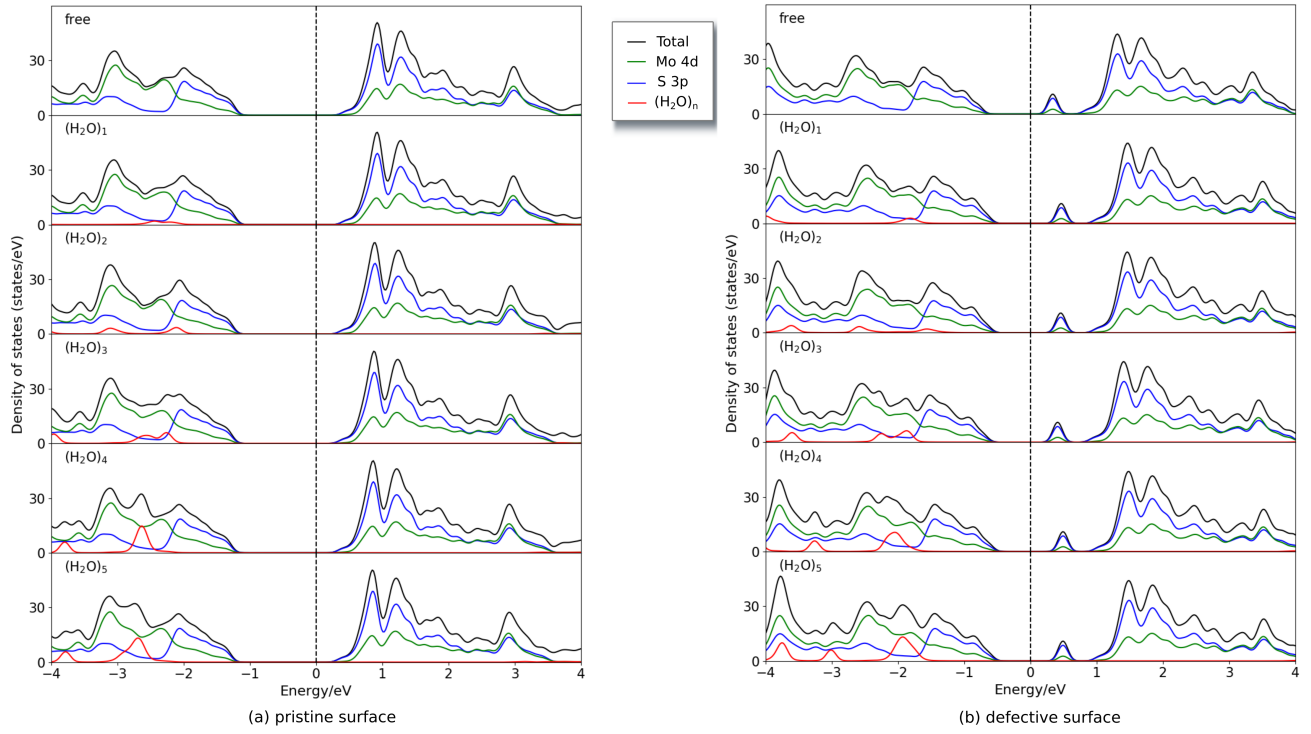


Figure S4. Total density of states and the projected density of states for $(\text{H}_2\text{O})_n$ ($n=1-5$) on pristine and defective MoS₂ monolayer by vdW-DF-cx functional.



Optimized geometries considered in this work (POSCAR format)

(a) Optimized geometry for (H₂O)₁ on pristine MoS₂ monolayer:

Mo S O H

1.0000000000000000

12.7335259874836861 0.0000000000000000 0.0000000000000000

-6.3667629937418431 11.0275569849102020 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.1729065632692084

Mo S O H

16 32 1 2

Direct

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0.5004129689188801 0.9999216811120348 0.4276561802671068

0.7503456862193545 0.9999478607999208 0.4276709583042617

0.7503788561748124 0.2498964890202657 0.4276726767268073

0.7504082284357452 0.4999904263967778 0.4276813359063851

0.7504221723760551 0.7499985481206153 0.4277012754927938

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0.2503830255654620 0.9999004142076515 0.4277041406638915

0.0003939201375474 0.4999839096315384 0.4277062345190714

0.2503943461173179 0.2498751549205807 0.4277160828598952

0.5003675104895748 0.5001455799817762 0.4277203544982555

0.0003404101698905 0.9999143258111189 0.4277293223269965

0.2506440309247964 0.5001940536374292 0.4277305820973538

0.0003914046148878 0.7499809115760669 0.4277314121676099

0.4170512265374455 0.5832721338734856 0.3538098260441842

0.4169478771790054 0.0830008926049928 0.3538484379842828

0.6673222494262419 0.3333791975893305 0.3538564487408351

0.4169490901305366 0.8333841143215679 0.3538591119557282

0.6672593329501240 0.8334071198703370 0.3538639852120085

0.9169614153826586 0.0831427167644279 0.3539166742935365

0.4170533079563583 0.3333447215036003 0.3539178311965756

0.9169830892809969 0.3333365307501879 0.3539179139910686

0.6670484133887626 0.0832663503128117 0.3539193530943834

0.1669822402951908 0.8332644399456584 0.3539610877517063

0.9171049752732188 0.5833761752311091 0.3539612103139973

0.9170897983547022 0.8332942393835978 0.3539659836784708
 0.6670268757312527 0.5833270103072081 0.3539863242490355
 0.1670953317123889 0.5833256231459316 0.3539934063187360
 0.1671166391094729 0.3333450345375795 0.3539948166116460
 0.1670247863236298 0.0832550399201111 0.3539986916582620
 0.4174229017854714 0.3331045848166099 0.5011596588447631
 0.1668142605474827 0.3332349196679232 0.5012620906952705
 0.6669840296749712 0.3332172421351487 0.5013378039656828
 0.4171697596055708 0.0833230985119684 0.5013565746525899
 0.6668845792779976 0.8332205700295319 0.5013658312938247
 0.4171417584001489 0.8332257485110475 0.5013709165663514
 0.4173534977289819 0.5838383581975606 0.5014046899171163
 0.9170189269514069 0.3332589248941389 0.5014062659879244
 0.9169486265894804 0.0832669201579748 0.5014209668509864
 0.6670030751244411 0.0832216572769298 0.5014654397247114
 0.9170379939367876 0.5833012482095441 0.5014693244062869
 0.1670605754751762 0.8332795792009051 0.5014761486937118
 0.1670441556001023 0.0832208214617083 0.5014810615761078
 0.9170125309346560 0.8332581019144740 0.5014833989972800
 0.6670331820230970 0.5833402987445453 0.5014839685931420
 0.1671354219822234 0.5833743385595724 0.5014871188455530
 0.3425268697175596 0.4204220439163535 0.6433309469957251
 0.2579256852375167 0.3717525896814351 0.6302465592111659
 0.3778248896119578 0.3702441059780455 0.6321601982233176

(b) Optimized geometry for (H₂O)₂ on pristine MoS₂ monolayer:

Mo S O H

1.0000000000000000

12.7335259874836861 0.0000000000000000 0.0000000000000000

-6.3667629937418431 11.0275569849102020 0.0000000000000000

0.0000000000000000 0.0000000000000000 22.2171660419423347

Mo S O H

16 32 2 4

Direct

0.5012764434112498 0.5020768547898911 0.4262267256374201

0.2511943660525020 0.2517387147306209 0.4266621034431139

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0.5011169536784266 0.7521174317529500 0.4268310217917843
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0.0012120808673615 0.0018604842421652 0.4268874961862963
0.7511846368701285 0.0018226649862285 0.4268985893202952
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0.0011163633293023 0.7517735216733996 0.4270471981929944
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0.6678473249287720 0.3349877667424366 0.3565376082640768
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 0.3426892808030502 0.5860351958138281 0.6276333697860323
 0.3401695084552614 0.6974089490105371 0.6547965362700339

(c) Optimized geometry for (H₂O)₃ on pristine MoS₂ monolayer:

Mo S O H

1.000000000000000
 12.7335259874836861 0.0000000000000000 0.0000000000000000
 -6.3667629937418431 11.0275569849102020 0.0000000000000000
 0.0000000000000000 0.0000000000000000 22.2171660419423347

Mo S O H

16 32 3 6

Direct

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0.6694188552429878 0.5844221178651665 0.4932665453060565
0.9196017005219659 0.3345168122048960 0.4932681175137787
0.9196162062098026 0.0845401565619355 0.4932684159316807
0.9194224228663614 0.5842492833014816 0.4932900739594928
0.4194478747105350 0.8341565725379851 0.4932970248910209
0.6695468808434839 0.3343796629702922 0.4933179479015948
0.9195015645715472 0.8343382428755532 0.4933199931669492
0.1695321829249039 0.3346170605193279 0.4933241314085137
0.1694578927059851 0.0843333694192268 0.4933395226604560
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0.1694849827747191 0.8341817706848076 0.4933663474138470
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0.5678122251952047 0.7068147898637633 0.6339931678688799

0.4104412642480852 0.4592678525198508 0.6345112875056671
0.6132187330173124 0.7615612257993121 0.6009625905839755
0.4119452403385822 0.4088378390761704 0.6017528988513234
0.4870414774582770 0.5381926951836391 0.6307869776704820
0.3254271584270043 0.5392207990524795 0.6334346483900006
0.4876178212546378 0.7022248628228738 0.6340093116920542
0.2755867985112133 0.6099935671341044 0.6702560935039088

(d) Optimized geometry for (H₂O)₄ on pristine MoS₂ monolayer:

Mo S O H

1.0000000000000000

12.7335259874836861 0.0000000000000000 0.0000000000000000

-6.3667629937418431 11.0275569849102020 0.0000000000000000

0.0000000000000000 0.0000000000000000 22.2171660419423347

Mo S O H

16 32 4 8

Direct

0.7487367619058602 0.4971323750583778 0.4192888682298204

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0.7489344729893759 0.2471798724531524 0.4195717152404654

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0.9985681314017256 0.7471826235198620 0.4196073880620332

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0.9985994747162721 0.9970562582406615 0.4196562498294654

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0.2487702855174589 0.4973249647682181 0.4196637364278715

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0.7486276323051229 0.7469821772194720 0.4197756801832284

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0.4153030176842591 0.0806569671067763 0.3492141802583291
0.6653340460649204 0.5806812382617821 0.3492271580161272
0.4154731378276679 0.8305892452456547 0.3492636038435819
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0.1651433084031666 0.8305449215572196 0.3492955299676694
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0.9155761343704754 0.3304621837807389 0.3493077034374750
0.9155024339055302 0.0805425416722301 0.3493186575348446
0.9150716528225544 0.8303851752958806 0.3493940778650853
0.1653006521931957 0.0805520731577758 0.3493996887067112
0.1654320933802182 0.3305802658728823 0.3494083455263848
0.4153616102004634 0.3306391819139307 0.3494288765427669
0.4154318899246690 0.8308062600389832 0.4894735799998244
0.6656849018168955 0.3307167830545268 0.4897548971573826
0.9151488345937793 0.5803681789862978 0.4897840246347016
0.6655103714056025 0.0804701382377147 0.4898252657182098
0.6657019993782782 0.5801249656432503 0.4898273087330551
0.4154840337490882 0.3305312109461482 0.4898345000192705
0.1652448724358209 0.8303618634236045 0.4898390559558763
0.4155186605428867 0.0805915666739310 0.4898431644906864
0.4155569925220703 0.5807410384515137 0.4898712162232428
0.1652461429683640 0.5805774789249156 0.4898860916578229
0.6654634693230506 0.8306233856269287 0.489888543864217
0.9152492505749876 0.0803824420234633 0.4898914726321451
0.9155571033608894 0.3306241634469984 0.4899373736259136
0.1652591570561839 0.0804001701567501 0.4899378880929675
0.1654314664315777 0.3307065369047990 0.4900048912380655
0.9152690132965091 0.8304268040991261 0.4900663122130666
0.6011762081985452 0.6557580909257865 0.6252616239971829
0.2592096048592154 0.5293256043915662 0.6333179719428301
0.4575571713732813 0.7520653528563486 0.6340869449057962
0.4042994395132240 0.4338213574907215 0.6415149003744816
0.4530275337966359 0.7988793215083732 0.6003195229680145
0.4007992954875448 0.3799148540998587 0.6093028406253254
0.5564879218008514 0.7024777443998005 0.6279174897313027
0.3771835903258349 0.6744772760800686 0.6345032509271178
0.4839270984834201 0.5109256609337649 0.6360260351533427

0.3041682956784300 0.4830622584212705 0.6367259007424337
0.6614026817857805 0.6877857719872651 0.6573893485077065
0.2051457706047870 0.5048115130683541 0.6680145317355937

(e) Optimized geometry for (H₂O)₅ on pristine MoS₂ monolayer:

Mo S O H

1.0000000000000000

12.7335259874836861 0.0000000000000000 0.0000000000000000

-6.3667629937418431 11.0275569849102020 0.0000000000000000

0.0000000000000000 0.0000000000000000 22.2171660419423347

Mo S O H

16 32 5 10

Direct

0.2489531089600021 0.7458827024084016 0.4188472050660863

0.7488381218714224 0.4957759513431768 0.4189574962670122

0.9988466474532416 0.4958293102438347 0.4190218391699148

0.2486356284028517 0.2457422948885792 0.4190220420878887

0.4990167953337306 0.9959918840292659 0.4190221682230586

0.4990996478986034 0.2458015044906077 0.4190613618410239

0.7489628126191192 0.2457703909542417 0.4190759726398241

0.9989525499892267 0.2457907410087543 0.4190915613574262

0.4990653312379294 0.4961868667587765 0.4191229593285968

0.4990930088695862 0.7459674571979491 0.4191298411211477

0.2489515610126176 0.9959500772819752 0.4191360744677652

0.7488742055719300 0.9957171522215589 0.4191462632577156

0.9988723012618621 0.7458320212327862 0.4191553358523095

0.7488395514034210 0.7457623722844673 0.4191776440393724

0.2489745586400716 0.4957790276278615 0.4192082133536559

0.9988378614929658 0.9957732383204885 0.4192337934521930

0.4158316504348321 0.8293147292524736 0.3487148697130849

0.1656019529928727 0.5789832982693284 0.3487480425562808

0.6656002202389644 0.3290003679322666 0.3487562010913550

0.6655248355115191 0.5792673312549326 0.3487839162213007

0.9156823567674977 0.5792985497133500 0.3487883514045578

0.1654946846978831 0.8293122760362905 0.3487986597150510

0.1655607909449088 0.3292627443223850 0.3488026183822441

0.6657025144595892 0.0791337704070827 0.3488058691356954

0.9156514376947058 0.3291458999133638 0.3488126287501316
 0.4155602789629356 0.0792387153560981 0.3488220803909670
 0.6656659073108315 0.8291258476909391 0.3488272231536556
 0.1653544043371795 0.0790513255358647 0.3488620895383221
 0.4155774191616075 0.5792947452698485 0.3488691222468887
 0.9155858146971951 0.0790446110150640 0.3488717162866877
 0.4156391564568693 0.3293220273368576 0.3488803407109913
 0.9155516980648812 0.8291923483821861 0.3489501225726102
 0.4156007390374299 0.8294123550284951 0.4890974907492165
 0.4155825130025832 0.3291220779462805 0.4891030191583923
 0.1654235663195323 0.5791855381578301 0.4891843316568938
 0.1654600704123581 0.3289053095462293 0.4893075689478366
 0.9153917826750799 0.5790569205516718 0.4893361074854212
 0.6657007668271504 0.3292035779134750 0.4893462970422462
 0.4157205527111074 0.0792223040164046 0.4893467321533578
 0.6656781803364211 0.5789858772593348 0.4893585924303707
 0.1657206419890471 0.8291377569891267 0.4893594292787782
 0.9156304503678001 0.3292095506335571 0.4893721977871763
 0.6655220562763446 0.0791266271643991 0.4894288563545928
 0.1655827820980420 0.0792595835973060 0.4894332852264611
 0.6656882576534073 0.8291728463888859 0.4894423744007668
 0.4157453857267441 0.5795286277067291 0.4895095813431354
 0.9154304964311066 0.8290180674584420 0.4895124745467925
 0.9155102722504509 0.0791444179618281 0.4895249028607580
 0.2341311872566934 0.4640374672501935 0.6257744767024676
 0.6223636050206096 0.6750259793538049 0.6330516400703772
 0.5349520386517312 0.8268028912800176 0.6334048757400552
 0.4363849478953341 0.4499553146130424 0.6338566701952786
 0.2930093556616740 0.6949528526249367 0.6339838317576465
 0.4335141231249580 0.4010733853489086 0.5992613518512826
 0.2654914301741371 0.7222164842642727 0.5994878921436992
 0.2535412286427388 0.5512364321532743 0.6291036769299723
 0.3586898446131883 0.4527477566288880 0.6317036906393483
 0.5533278460185329 0.5879902187555146 0.6335331279351095
 0.3841750678948799 0.7472308295508299 0.6338715578067706
 0.5719236811801096 0.7728711115117903 0.6356592891815396
 0.1732289560454277 0.4199051170243635 0.6566106631962754

0.6798008423100796 0.6791298968030759 0.6632542562849792
0.5685264430545658 0.8823768790517903 0.6673516853629380

(f) Optimized geometry for (H₂O)₁ on defective MoS₂ monolayer:

Mo S O H

1.0000000000000000

12.7335259874836861 0.0000000000000000 0.0000000000000000

-6.3667629937418431 11.0275569849102020 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.3797881478684886

Mo S O H

16 31 1 2

Direct

0.4987104480172562 0.4970976913172009 0.4640276768240312

0.4987594091452934 0.2538452658611163 0.4641316345995676

0.2552468459268056 0.2537664985231842 0.4641458247366188

0.7482450119688764 0.5001884468209425 0.4656594174554911

0.2523695533309862 0.5000717595847490 0.4656830772795999

0.2524403020284609 0.0045694107868357 0.4657172670145400

0.2515236075107410 0.7518760639315687 0.4668196484754219

0.0007606281990817 0.5010753583589960 0.4668247106672609

0.0007534416352897 0.7519054435885764 0.4668334373744116

0.5009355254676393 0.7506949587686478 0.4672458180566181

0.5009375835299466 0.0024945491209678 0.4672761775914225

0.0018959494771522 0.2516661837677105 0.4673155326726786

0.7501595746670304 0.7507618688361504 0.4673318428634872

0.0019108826779686 0.0024729599789239 0.4673392090812385

0.7501452070739916 0.2516465683745608 0.4673531319780224

0.7510151804677250 0.0016255029569621 0.4678617306902737

0.4174815292203533 0.3348006659549370 0.3870933179068530

0.4196135112531039 0.5852523860979204 0.3890235194295784

0.1672181404539046 0.3328424798684182 0.3890468332875514

0.4196510537220632 0.0866435252624029 0.3890751304275923

0.1672186652902568 0.0865650501200506 0.3890791858104876

0.6660596452792618 0.5853334664332763 0.3890844274899550

0.6660006312115172 0.3328726191543723 0.3891030273317995

0.9174920218210332 0.5848510843767087 0.3902020074744854

0.1678108919730548 0.5847718140833393 0.3902286108138924

0.1678252429972389 0.8352878752363040 0.3902656114499194
 0.4186365462651054 0.8354700860814006 0.3907067110214868
 0.9171598416773250 0.8354743478370068 0.3907623382243344
 0.9171186420881696 0.3339029495124279 0.3907639472378293
 0.6677957071512637 0.8351387149795571 0.3911059188484813
 0.6677941338577753 0.0848926450628014 0.3911397423202274
 0.9174887839698087 0.0848441587492559 0.3911519474132277
 0.6617879539117624 0.5786828213509310 0.5423053614932769
 0.4173379810137874 0.5787355134459276 0.5423054523331814
 0.6617626682679756 0.3352983786594166 0.5423491732313650
 0.1737295630820981 0.3351535050834258 0.5423648139924211
 0.4173979274978024 0.0908474961552059 0.5423654763467525
 0.1737734694324544 0.0908573681341096 0.5423961294124240
 0.9158195105879656 0.5840078912294331 0.5427003050742201
 0.1686689172968272 0.5839391469069781 0.5427095497725247
 0.1686884612825423 0.8369911224975652 0.5427290912617906
 0.4173095021123601 0.8347749428107463 0.5438081457015826
 0.9179042259315509 0.3353319164021542 0.5438763966544542
 0.9179031413969412 0.8348106937201365 0.5438789642761179
 0.6671564988436884 0.8340544997914492 0.5441734567577328
 0.6671831067789640 0.0853789351395662 0.5442186938357736
 0.9186182392828215 0.0854398779656833 0.5442459531058219
 0.3955634876241021 0.3180466996198064 0.6464217681641600
 0.4206539780493372 0.3395659170529726 0.6006061055398249
 0.4629519670047841 0.3809005089702282 0.6715778153331371

(g) Optimized geometry for (H₂O)₂ on defective MoS₂ monolayer:

Mo S O H

1.0000000000000000

12.7335259999999995 0.0000000000000000 0.0000000000000000

-6.3667629999999997 11.0275569957496469 0.0000000000000000

0.0000000000000000 0.0000000000000000 22.2171659999999989

Mo S O H

16 31 2 4

Direct

0.5106196391927398 0.5044137857855020 0.4212884361109133

0.2669804114322787 0.2604392795252579 0.4215322582684422

0.5104457759197700 0.2603491042497694 0.4215443586476582
0.7597711140203458 0.5065792575497454 0.4222514831076438
0.2638389510845869 0.5067214306594252 0.4223282286044565
0.2640495647837966 0.0110381995711251 0.4230473482899129
0.0123530224951409 0.5077147048299082 0.4237006837375077
0.2631278082044801 0.7584935235445585 0.4239003888088249
0.0123214509925447 0.7584763036413307 0.4239051885587131
0.7617054277068291 0.2581120255838769 0.4242090021260410
0.0133037242024869 0.2581095821650052 0.4242541259328547
0.5125217505491406 0.7573205924844757 0.4242802081618464
0.7616212529609570 0.7572597752117645 0.4242947648084510
0.5125062408423702 0.0090184923518137 0.4244158431568934
0.0134150070187928 0.0090546106531164 0.4244748424197695
0.7624480116166623 0.0079829012718804 0.4247736715466388
0.4292975082337946 0.3416141815186720 0.3510093475474108
0.4313803580126461 0.5921253397708881 0.3522251190461390
0.6776144693992023 0.5921050879890188 0.3522392470305107
0.6772286779009065 0.3390186946004334 0.3523788843724134
0.1787723694006189 0.3391047687258961 0.3524502305814892
0.4311565715451380 0.0932094838739701 0.3527111954044813
0.1789872085252995 0.0932037690240790 0.3527725093643781
0.9293409078222723 0.5916972187771208 0.3533783288406482
0.1793450849267231 0.5917001792170780 0.3533894713011918
0.1794949585226533 0.8420459923538743 0.3537165052478670
0.9287352138744893 0.3404921622869708 0.3539767054253815
0.4301591105938556 0.8421344860199298 0.3540997061036961
0.9288649787062866 0.8421538733476766 0.3541578033318800
0.6792760097317441 0.8416173456521534 0.3543649221035992
0.6791352480078956 0.0912187964930027 0.3544255270069883
0.9290503880992560 0.0912485318206890 0.3544608561431559
0.4283459983210776 0.5854087335656999 0.4926259911554212
0.6737789968024330 0.5851222742828810 0.4926424308334205
0.6738711232013443 0.3421753405863726 0.4930263196042830
0.1852665945241441 0.3423050247998560 0.4930410743926004
0.9269349392657489 0.5902741293530127 0.4932808380976823
0.1803047967908142 0.5903703975210846 0.4933106145331649
0.1853303771959958 0.0973077201485495 0.4933373045029157

0.4290564668280510 0.0973216486709774 0.4933390241781481
 0.1801620540820608 0.8432976731255621 0.4935824955121788
 0.9293779950949030 0.3419256663313419 0.4943968704798962
 0.4289238558879589 0.8412327146416843 0.4946175678755225
 0.9291884628403650 0.8411686697775878 0.4946176025693489
 0.6788997175384424 0.0919071319856855 0.4948720179868644
 0.9298373223206085 0.0919070049656909 0.4949032721740281
 0.6786507425907971 0.8405180000809764 0.4949171809190034
 0.4431218801627281 0.3670799146155090 0.5911380716425683
 0.5665497390545013 0.6280640493920089 0.6116796537954485
 0.4344665966692105 0.3521992913454426 0.5475099170608502
 0.3604527530601516 0.3197631111722714 0.6065442016679725
 0.5246083285989300 0.5387569497339513 0.6080793519221004
 0.6421544429371124 0.6492257839623718 0.6323962614808494

(h) Optimized geometry for (H₂O)₃ on defective MoS₂ monolayer:

Mo S O H

1.000000000000000
 12.733525999999995 0.0000000000000000 0.0000000000000000
 -6.366762999999997 11.0275569957496469 0.0000000000000000
 0.0000000000000000 0.0000000000000000 22.217165999999989

Mo S O H

16 31 3 6

Direct

0.5080797555457579 0.5018627986783386 0.4038328545432819
 0.2643181314887784 0.2584380473046011 0.4039028485556884
 0.5080318918254036 0.2585477181146274 0.4039504744199647
 0.2615849019348317 0.5049719534019417 0.4049420730014859
 0.2616295918953426 0.0092151373420748 0.4052154804828803
 0.7572643510240837 0.5049421087873966 0.4053141142245735
 0.2606583280230979 0.7566415856122006 0.4063695136733472
 0.0099177677068383 0.7566313261116591 0.4064075063868060
 0.0098470349834372 0.5058080537051524 0.4064107613146319
 0.5102811508551923 0.7557506483196974 0.4067168943180164
 0.7591991693899516 0.7554032177607226 0.4068391078191951
 0.0110100849627770 0.2563795349314333 0.4068597956172937
 0.0109641707652059 0.0072860593832402 0.4069089961265249

0.5101378201936484 0.0072335701791530 0.4069337179175321
0.7592834274549674 0.2564118361980263 0.4069435061636284
0.7602873800301850 0.0064676351422435 0.4074667580378915
0.4267031082582093 0.3394701305523284 0.3333628478145201
0.1762011282526856 0.3373980448448606 0.3348805393164014
0.4291652793130112 0.5902468353899479 0.3349080159421547
0.6751917534973728 0.5900641520318430 0.3349838488682835
0.1762730990781876 0.0912351171922126 0.3350285612503612
0.4289808384545495 0.0913327846483796 0.3350743764271158
0.6752087128868283 0.3375984212785141 0.3350845094683237
0.1767770885932052 0.5896876871639520 0.3360079170102779
0.1769320995898980 0.8399345549572885 0.3360880186965360
0.9265388569094881 0.5895720460534974 0.3361247798219580
0.4277592676456123 0.8403773256993006 0.3365843235394621
0.9262254931216560 0.3386912422087747 0.3366423019464122
0.9263584014103614 0.8402272387262926 0.3366497142724754
0.6771818359382493 0.8402122571896911 0.3369708569361052
0.9265174563031806 0.0895841882732427 0.3370150463540824
0.6769429726063123 0.0895850092942965 0.3371221470932895
0.4265183476985328 0.5836700137503641 0.4752904629923691
0.1831544167304813 0.3403967510428458 0.4752946438506385
0.1829949065631311 0.0953884465303929 0.4755501749452762
0.6708473678716302 0.5833483653583045 0.4756943750382945
0.4263644572906742 0.0955447343836724 0.4757093158485688
0.6709653360732588 0.3401566667394604 0.4757372891797331
0.1779317703846957 0.5885629040209110 0.4758974017535067
0.9248145667966696 0.5887042896673478 0.4759838414110433
0.1778516380972803 0.8417452819977171 0.4759905809436376
0.9268847753129776 0.8394856338551051 0.4770294745429311
0.4264643289246379 0.8394316003564057 0.4770312512267836
0.9270699526896209 0.3400556976315841 0.4771081262482113
0.6763816397502680 0.8387893970841844 0.4774257516732661
0.6764276553832360 0.0901791487296251 0.4775365067758628
0.9278554930533218 0.0903171738285948 0.4775815327293955
0.4170608660428101 0.3294854372383611 0.5809420760437689
0.1678355701277781 0.2262960120329396 0.6086330173739825
0.3248490648977551 0.4692018523723718 0.6258832628107598

0.4285442044020087 0.3282996421389939 0.5374001283733776
0.3304194350714411 0.2685343003751299 0.5876870393706000
0.3314158300289520 0.5341573106689950 0.6000369818570377
0.3815172962429259 0.4450563880622340 0.6082199494586504
0.2025593679463213 0.3138654917625345 0.6185487961099199
0.1335220450385748 0.1830816826041115 0.6462376048968750

(i) Optimized geometry for (H₂O)₄ on defective MoS₂ monolayer:

Mo S O H

1.0000000000000000

12.7335259999999995 0.0000000000000000 0.0000000000000000

-6.3667629999999997 11.0275569957496469 0.0000000000000000

0.0000000000000000 0.0000000000000000 22.2171659999999989

Mo S O H

16 31 4 8

Direct

0.5008802167746040 0.4999608279114156 0.4039946464864954

0.2571580897963202 0.2563197293282258 0.4041470946056265

0.5006721728746655 0.2563963662866513 0.4041784019732191

0.2543145903035580 0.5026688674843527 0.4050331651689163

0.7500020258638074 0.5026996617448631 0.4053481233041012

0.2543214409763834 0.0070652513611407 0.4056130065973775

0.0025299380062478 0.5035714993758518 0.4066807380842761

0.0026238622588153 0.7543921180551507 0.4066936854502714

0.2534225355080366 0.7544917606731403 0.4067804826281147

0.0037056280978263 0.2541536044592618 0.4070231860074074

0.7520237285292026 0.7533336582199226 0.4070807719520460

0.5029316676500315 0.7533617973806486 0.4070812932429178

0.7519607421689898 0.2542060229862386 0.4071634251873135

0.0037732212496451 0.0050297033555466 0.4071873411857396

0.5028044959786300 0.0051120761115939 0.4073177231400678

0.7528427193524649 0.0041285777070712 0.4078146135187097

0.4194959864634953 0.3374465438360446 0.3335811777659714

0.4219038178906658 0.5881837871172308 0.3350079192144477

0.1689756944234801 0.3351297907094590 0.3350216611195407

0.6680398553678586 0.5880676889532452 0.3351139086359112

0.6677248199621388 0.3352373532014212 0.3352336358027017

0.1691131290410510 0.0890696977718122 0.3353298881526001
0.4215842164624988 0.0891125086516240 0.3353885991656824
0.1695117820167482 0.5876456897667808 0.3362878440880124
0.9194397932760126 0.5874150105549774 0.3363229445210365
0.1697524725691011 0.8377845746588974 0.3364644685448752
0.9189443639168786 0.3365278421239069 0.3368749950854308
0.9191703846416104 0.8380377008217863 0.3368778199910807
0.4204805859122231 0.8381841984905307 0.3370244377007978
0.6697835326779753 0.8379774422480253 0.3372919464467046
0.9190965828691446 0.0871600138536266 0.3373326706395119
0.6695448972739513 0.0872895554805027 0.3374514240201592
0.4189052540122304 0.5810711324766302 0.4754069923966853
0.1758189816545439 0.3382030499823827 0.4754788768297686
0.6638731055497971 0.5813741627254529 0.4756991182939601
0.6637865178141595 0.3380893583195004 0.4758896096482559
0.1757796288457101 0.0934471855870171 0.4759599794279978
0.4190727217371659 0.0935193642548100 0.4760640598052035
0.1707407467996234 0.5861777386531557 0.4761370382289840
0.9173074593137542 0.5863537432409345 0.4761863660960941
0.1704890399469434 0.8395350109241519 0.4763280412292943
0.9197374968398933 0.3377500647306704 0.4773274298071684
0.9196226489667580 0.8372583035310228 0.4773293233755069
0.4192690678646471 0.8372257381627648 0.4774565425488362
0.9206186176947071 0.0880846197914238 0.4778034767083952
0.6690128083297040 0.8363713503638621 0.4778230420106482
0.6691112340973646 0.0880960914526909 0.4778595129325183
0.4490265894829548 0.3618201484405361 0.5836993772570125
0.5111376731774584 0.5897063919761365 0.6159225819632610
0.2164658423109955 0.2798043379403055 0.6169233633045152
0.2708920005584829 0.5120565018161258 0.6255680252508355
0.4486632625562947 0.3445746691217693 0.5407567373776487
0.2457819311178469 0.5479490417682413 0.5938718973808790
0.3612227056721977 0.3206880025567784 0.5957393845524663
0.4993475498273696 0.5086070672241263 0.6031270166664697
0.2254251958363511 0.3626929698206567 0.6209864992445162
0.3615923652796553 0.5525084168715821 0.6227391294131976
0.5601278653520438 0.6113139536197352 0.6524204334173831

0.1904728554038329 0.2420392419553181 0.6563916434235324

(j) Optimized geometry for (H₂O)₅ on defective MoS₂ monolayer:

Mo S O H

1.0000000000000000

12.733525999999995 0.0000000000000000 0.0000000000000000

-6.366762999999997 11.0275569957496469 0.0000000000000000

0.0000000000000000 0.0000000000000000 22.217165999999989

Mo S O H

16 31 5 10

Direct

0.5117900553082251 0.3568287974309499 0.4040100760215495

0.2683697884966207 0.3570726598488960 0.4040121452817544

0.5118416801035934 0.6003825442439137 0.4040393163410982

0.2655769134497135 0.6034047749537876 0.4051494327171952

0.2655036356003606 0.1076171006671132 0.4052685599757027

0.7613434317658800 0.6034079042560805 0.4053548014385129

0.0139635444994752 0.6042865580753585 0.4063682672841153

0.0140729821192593 0.8550493810103390 0.4064163783156829

0.2646446332818400 0.8549788934034623 0.4065695554075361

0.7633023400182637 0.3547477651383488 0.4068531208966490

0.5140594098076292 0.8537971828693856 0.4068550186860804

0.0150219840780466 0.3547851540131077 0.4068942552609016

0.0151011656095363 0.1057770138435927 0.4069090096356476

0.7632388370366385 0.8538725723204337 0.4069897221264611

0.5139251120308970 0.1055100472041133 0.4070575589197958

0.7641812398680301 0.1046946792797740 0.4075373213375002

0.4306830345566510 0.4380435497763315 0.3334905552423209

0.4329264590208481 0.6884415289585988 0.3349788638602007

0.1803555446785339 0.4359792818580033 0.3350028327342613

0.1804200878685478 0.1898817951377296 0.3350251563430930

0.4328051157423971 0.1896785402425039 0.3351028607737661

0.6790048046078425 0.4359651096291017 0.3351104014135728

0.6791110592302374 0.6885078564390099 0.3351920151571619

0.1809923450620801 0.6882232236509225 0.3360622390367141

0.9305866651197263 0.6880187727327822 0.3361185965953624

0.1810921273167025 0.9383365121553382 0.3361619044221271

0.9303122314216452 0.4371099171675610 0.3365705738788876
0.9303748722307859 0.9386444603019584 0.3367095877625985
0.4316675679347597 0.9385872455153219 0.3367434508112339
0.6810105215425679 0.9383996319673145 0.3370703311156760
0.9304760637777392 0.1878871708267766 0.3370752187429176
0.6807430543079462 0.1877202501615045 0.3371768480419846
0.1871677533301934 0.1941438640912452 0.4755077718615439
0.1870267099630993 0.4388019914993038 0.4756091521268360
0.6750978593532935 0.4384555220255493 0.4756386732519573
0.4300822775964477 0.1939408613577740 0.4756430021197176
0.4301961142584503 0.6818498340311905 0.4757073842767880
0.6748849563175341 0.6818412636778106 0.4757596547038716
0.9290046937945178 0.6871180678983606 0.4759900103735717
0.1817717532707519 0.6868581300211858 0.4760437170737148
0.1818333621251540 0.9401310770026186 0.4761052266539565
0.9310027127855918 0.4385132544937704 0.4770303815586345
0.9312018364318462 0.9380408550700210 0.4771207948287000
0.4304958419919274 0.9376769896929531 0.4772297598387709
0.6801114679450393 0.9369832985003725 0.4775433567438014
0.6803851675261257 0.1886242263088178 0.4775807338916280
0.9318952449497715 0.1886739876875865 0.4775982164567267
0.4276652981249782 0.4393010739846019 0.5812861803926168
0.1970524601730830 0.3088694548218669 0.6167108839321287
0.3573101491355288 0.0804144285990702 0.6239703260542555
0.5302219026223227 0.3150755061593387 0.6248442200700808
0.1474321545467205 0.0793821362879470 0.6252705104848530
0.4351088675903938 0.4431942811808582 0.5373770202181092
0.4711774679024003 0.3957888145098352 0.5952288207023884
0.0839168643093231 0.0323399412837304 0.5960105766487516
0.2846226331506401 0.3611957838647655 0.6040641974071193
0.6025258905090070 0.3230959934211910 0.6054076030138731
0.1623902559385115 0.1648862055175755 0.6225256600154836
0.2760630884477990 0.0763520792195536 0.6230347005281018
0.4688766068125929 0.2256655374959209 0.6247460162125975
0.1882575519117609 0.3456139301028003 0.6534528138152425
0.3556564169295982 0.0370478788734161 0.6604476704953157