

# Finding the catalytically active sites on the layered tri-chalcogenide compounds $\text{CoPS}_3$ and $\text{NiPS}_3$ for hydrogen evolution reaction<sup>†</sup>

Khorsed Alam,<sup>a</sup> Tisita Das,<sup>a</sup> Sudip Chakraborty,<sup>a</sup> and Prasenjit Sen<sup>a</sup>

## Supplementary Information

### POSCAR Files

CoPS3-R2

1.0000000000000000

29.7119350432999987 0.0000000000000000 0.0000000000000000

0.0042066790000000 10.2238255429000002 0.0000000000000000

0.0068087461000000 -0.1473233373000000 18.9304939453000003

Co P S

12 12 36

Direct

0.3013483370539047 0.1667645774008412 0.4950735337216705

0.4998477243993406 0.1701958624878559 0.5015116378948264

0.6913742470069707 0.1806451904478712 0.5058007385404863

0.2102167812725400 0.6799525019828825 0.4896709536983477

0.4016723963612098 0.6701923011568339 0.4955197101340765

0.5999725707984370 0.6676568910895446 0.5018255638603775

0.2101744056962098 0.3240147448065416 0.4893048780043330

0.4016173390893531 0.3348364762207456 0.4958975638758514

<sup>0a</sup> Harish-Chandra Research Institute, HBNI, Chhatnag Road, Jhansi, Allahabad 211019, India.

0.6001179922692605 0.3379627702230953 0.5017000566854619  
0.3014679414318586 0.8374358624391316 0.4949462821263833  
0.4997589879475242 0.8347294418423599 0.5011267631897396  
0.6913161813910016 0.8247773970907196 0.5056817957179026  
0.2008813769598146 0.0013641549094548 0.4482532714233495  
0.4014399363044673 0.0020623822208462 0.4412744436263875  
0.5994011382634009 0.0019123226777845 0.4484508828545867  
0.3038467860094919 0.5012109583237798 0.4324732022196304  
0.5015771841054599 0.5012666514222694 0.4408817795334317  
0.7066295156629653 0.5017746757823029 0.4326864565061214  
0.1945193857065853 0.0030463325660323 0.5627708605218246  
0.3999192518651858 0.0034455021702916 0.5567253899806693  
0.5978936387310125 0.0034811712143431 0.5637791930022840  
0.3017839832337612 0.5025872078252603 0.5478226573325943  
0.4999722220672432 0.5030164074283578 0.5563110510144957  
0.7008949603617856 0.5034735626260570 0.5472747729085128  
0.3681406031281571 0.1691553813825871 0.4144492097680635  
0.5678456961272755 0.1687974142577444 0.4192041620703511  
0.1704275718312085 0.1725532252414463 0.4186051034608860  
0.2706398982205417 0.6684776239282774 0.4057489427594105  
0.4683163293892263 0.6703217884691264 0.4154464602716811  
0.6655339685322034 0.6732742285521404 0.4207216125806143  
0.2704790322753046 0.3339593788538515 0.4052096210199908  
0.4684340231761011 0.3311712132622199 0.4157800426955120  
0.6656741576803951 0.3298738401416991 0.4207383742679517  
0.3682780203797648 0.8339731487418245 0.4142934130770854  
0.5677677917970928 0.8342794048722598 0.4192412313225226  
0.1704482462817238 0.8287252538993531 0.4191243712385428  
0.3714532781437234 0.5009390098432691 0.4122575134538541

0.5680459162351217 0.5014928594132481 0.4156195285727644  
0.1672912659331730 0.5020812632382106 0.4689694668838862  
0.2689038930773161 0.0009924408999817 0.4198578951870732  
0.4687989217823131 0.0015301990982687 0.4180175429621718  
0.6720086804414217 0.0016966755757745 0.4350023992836625  
0.3333159028981364 0.3357942868496740 0.5774948137365564  
0.5333582813058294 0.3359622386541758 0.5829634004390656  
0.7315058426315403 0.3319290619902041 0.5761852719148469  
0.2355810226276721 0.8313309641766263 0.5752100985804751  
0.4331675325416173 0.8340605518846707 0.5815188214824079  
0.6313406300474411 0.8368590215499557 0.5905612476343171  
0.2355144765586284 0.1747804988856131 0.5751842877952604  
0.4329907948282665 0.1734999904873651 0.5818849707321264  
0.6312589147974679 0.1712462704268097 0.5903849552551746  
0.3333715012272231 0.6704862867555460 0.5769438784815973  
0.5330507933246226 0.6714222340488356 0.5828581282278072  
0.7315812039174467 0.6759156066994954 0.5759033064757257  
0.3333561345474895 0.0029663878889920 0.5818439022450261  
0.5303710978620058 0.0033930632459820 0.5844638238811306  
0.7343875662502484 0.0026320429230955 0.5249497187343236  
0.2290852470006845 0.5028610533290526 0.5601529207683157  
0.4325518263498899 0.5040500744341961 0.5790274249984163  
0.6329579082803863 0.5040218964135365 0.5764248518186139

NiPS3-R2

1.0000000000000000

29.4447975158999995 0.0000000000000000 0.0000000000000000

0.0009544936000000 10.0675916219000001 0.0000000000000000

0.0180823273000000 0.0138533164000000 18.7848792246999992

Ni P S

12 12 36

Direct

0.3030904244584558 0.1677584007443255 0.4947744895046333

0.5001489512890878 0.1693885430198926 0.5008586762766718

0.6929419040714946 0.1834060433998774 0.5056760692501320

0.2105725702263752 0.6830457315308398 0.4920606688253684

0.4013840597709841 0.6701431538488609 0.4963280787157573

0.5985478565006256 0.6655804239694004 0.5009717468820150

0.2100726572808454 0.3261522118850867 0.4918319911865133

0.4014352339310593 0.3356146567944590 0.4968228659544169

0.5985081041917923 0.3367183084122981 0.5010823169549575

0.3024689762824751 0.8394431699265975 0.4950773340179084

0.5000829376383894 0.8346305079189335 0.5006378090777067

0.6930005764807371 0.8182416848637208 0.5059220355326455

0.2017912971382943 0.0044774834888173 0.4500620963935745

0.4024522870267425 0.0028273953819926 0.4404117264737848

0.6001699818527126 0.0014963266051393 0.4422180558727981

0.3033295942061838 0.5036634789916218 0.4334696219097599

0.5005644748189746 0.5019685738722203 0.4412018881607200

0.7045154481228605 0.5008644990085079 0.4318323952405920

0.1976514498989925 0.0048748378165678 0.5654981752641912

0.4009541067613092 0.0024426496787724 0.5562847986312885

0.5988654154813420 0.0006642063706763 0.5582052486151583

0.3017534652365182 0.5035641519081283 0.5495974395160647

0.4993272407469680 0.5020351168363620 0.5571334878248726

0.6996240480907292 0.5003868728832623 0.5475750648219235

0.3688715084469884 0.1734133095716469 0.4146732854012368

0.5659547771492092 0.1720971443281872 0.4186880645260471  
0.1705964852895646 0.1788283134061917 0.4209482832306512  
0.2704276641082828 0.6756824746292396 0.4072181398728972  
0.4669403861811975 0.6739206269959460 0.4165355317367202  
0.6628364753069432 0.6735375675441656 0.4212414691534348  
0.2708634005167875 0.3300904044293383 0.4084467657833076  
0.4669399913629472 0.3301118810454339 0.4167155031917759  
0.6626901215671372 0.3288211232181778 0.4209762085439608  
0.3686309779538052 0.8328695204390990 0.4149166630462235  
0.5659002164556578 0.8313377674452951 0.4183751117571503  
0.1705912995209377 0.8303753989474768 0.4213334923616131  
0.3715424062224675 0.5033452890702411 0.4132020951017392  
0.5677972096132182 0.5014614311469067 0.4166855958958435  
0.1704326904486511 0.5040955906364669 0.4629880032059601  
0.2701071358021128 0.0038359325933667 0.4193992787876179  
0.4703826354902975 0.0023344668458094 0.4179210016266123  
0.6843910943384107 0.0007395797036700 0.4391899250455273  
0.3343177125580366 0.3342927096771247 0.5779062742626486  
0.5329477063664476 0.3314741892212117 0.5829295765689085  
0.7313931559571966 0.3282329216261655 0.5776856250716307  
0.2388858812970955 0.8312618573028520 0.5754257577535589  
0.4343543133710304 0.8303885817745765 0.5812584689965725  
0.6314146883893638 0.8283512434812029 0.5856061208580763  
0.2394312918461194 0.1768494128438602 0.5755985377639020  
0.4345181149261246 0.1739871453063416 0.5814607994007098  
0.6314866593345055 0.1725393637759191 0.5856845746098037  
0.3337848842472061 0.6737568308923809 0.5776319343299697  
0.5331045589405176 0.6723332677706793 0.5824358170010576  
0.7313731611886930 0.6724287458592304 0.5778093297318945

0.3334421579330924 0.0033785985472833 0.5796293885525359  
0.5310129110456807 0.0010557361788756 0.5820551792402291  
0.7343316977064002 0.0008186366819073 0.5249393313108516  
0.2254594235070485 0.5037218909358719 0.5591105157203846  
0.4312912201845487 0.5027461925388442 0.5795898732108643  
0.6313439298402659 0.5004081684686758 0.5772684957070362

CoPS3-R3

1.0000000000000000

5.9039783477999999 0.0000000000000000 0.0000000000000000

0.0084133580000000 35.4476510858999987 0.0000000000000000

0.0068087461000000 -0.1473233373000000 18.9304939453000003

Co P S

8 8 24

Direct

0.5034111408863732 0.2157860717467379 0.4970374209535424

0.5022963992651792 0.5060998426287822 0.4995852715486008

0.0018292917308046 0.3620496875491651 0.4982317052294015

0.0008413310378137 0.6467038678001058 0.4981234154340613

0.0025418576086960 0.2661002902470205 0.4972896876811075

0.9989901106254652 0.5535305113703723 0.4996077433508420

0.5024616966252033 0.4098594039092265 0.4990150638110223

0.5006301419581729 0.6895343579501255 0.4975736127538863

-0.0001076690413338 0.1671115130678778 0.4379924578789006

0.0042963287955487 0.4579869967610071 0.4413056960326546

0.5044499741136503 0.3136016633985445 0.4402725342369013

0.5063702033703698 0.6017140536483616 0.4403244798673139

0.0070516194834852 0.1674235460194686 0.5552318133639338  
0.0026710839098717 0.4582124098502168 0.5566673562670061  
0.5001195322084341 0.3139334424533848 0.5553975089272871  
0.4964438431488696 0.6024263184295103 0.5568120689891906  
0.8171734367782769 0.2191507985553346 0.4241952032839901  
0.8375873067352354 0.5067096449201224 0.4158120763089553  
0.3347869999189894 0.3621224027983777 0.4154061350107892  
0.3432171802496686 0.6494980442853739 0.4090754812163922  
0.3414656798467220 0.2642374346840546 0.4151681959518933  
0.3365778691163672 0.5531763362190779 0.4159856609673884  
0.8343740736143556 0.4095711220966599 0.4156904972651522  
0.8742485743200386 0.7076041615907190 0.4572455196860218  
0.8418092406510197 0.3139585222648953 0.4154746241340517  
0.8425855883201893 0.6015167889448294 0.4154256073501362  
0.3374822028176565 0.1758051582489657 0.4161581057833784  
0.3418725734693084 0.4577457030251211 0.4165947778029969  
0.6643730048326925 0.2649123600701357 0.5799219040756900  
0.6675952971241400 0.5544214390586577 0.5826400534318599  
0.1697067784710632 0.4095918303720799 0.5815589415137893  
0.1256343269486360 0.7081271506379587 0.5372555896937455  
0.1886723205470228 0.2194698857038301 0.5694946895031635  
0.1695164144057818 0.5067292515607223 0.5832279921065959  
0.6686122038517587 0.3625146538137903 0.5816198387218170  
0.6587890061263065 0.6506950325907154 0.5870249494584611  
0.6701436883484269 0.1765193040362455 0.5777050780852778  
0.6650459710363026 0.4583369691583586 0.5813903836967813  
0.1622967667947686 0.3144899493637403 0.5798649524749504  
0.1588922437944656 0.6024619401528490 0.5815994795366141

NiPS3-R3

1.0000000000000000

5.8149323463000000 0.0000000000000000 0.0000000000000000

0.0019089872000000 32.1351832439000020 0.0000000000000000

0.0180823273000000 0.0138533164000000 18.7848792246999992

Ni P S

8 8 24

Direct

0.5027681889076472 0.2408923202739098 0.4983028793116833

0.5014945115441691 0.5525731024232655 0.4984391356607591

0.0026723534269637 0.3960546569837607 0.4979373655665178

0.0058955205830604 0.7055108684261490 0.4976599892607920

0.0026293614287139 0.2919302893062530 0.4979896579437107

0.0019846791828739 0.6044155396138517 0.4982313716350211

0.5016597009754385 0.4482130274729326 0.4981088608847136

0.5086235957926272 0.7522574095391005 0.4957673871237088

0.0026168155445084 0.1842623835843217 0.4397585790324874

0.0010659534016501 0.5002483198843067 0.4405349568515962

0.5049027354147282 0.3440420214373407 0.4399474444536391

0.5049192500580736 0.6570840575663687 0.4388938717744514

0.0029474069817925 0.1843462329993892 0.5575600779759755

0.0007669722674047 0.5002153558377040 0.5564351019621741

0.5007620336750365 0.3440534443569598 0.5557826297976588

0.4985599607411570 0.6572859890621789 0.5561812008765272

0.8178227024839005 0.2423821396422912 0.4250748097740731

0.8303459681772339 0.5539222542265501 0.4161596060313290

0.3309308067757555 0.3971701612097197 0.4147859461924276

0.3374694994552719 0.7094729895886041 0.4083893271946497

0.3360425836479036 0.2893473582142326 0.4166349801643116



0.3349559088078660 0.6030803654737102 0.4157857554342684  
0.8301224982008085 0.4466483802042049 0.4161184900113353  
0.8715811592838454 0.7686852650468938 0.4623927780716912  
0.8457834810376738 0.3444915353633888 0.4151468012105279  
0.8496464551257285 0.6572483564215695 0.4168133176785092  
0.3440059465151793 0.1934070475680479 0.4201479154746504  
0.3432160164421668 0.5001459751072055 0.4158351602603257  
0.6691707891050879 0.2893874912378273 0.5795754113444631  
0.6694365295923435 0.6035683310580334 0.5807067498364739  
0.1731340879556003 0.4466516531558734 0.5803728997981312  
0.1305996411205048 0.7685073683401270 0.5385281679546516  
0.1875883460724430 0.2425791350979801 0.5712813291281444  
0.1721237871699705 0.5537935969356459 0.5809779186733379  
0.6747293918901243 0.3971601691543254 0.5807327841061889  
0.6589671320373237 0.7106638078065360 0.5858092905024789  
0.6612125210413514 0.1934268472810931 0.5769811441132550  
0.6582553807730382 0.5002014411355570 0.5807852484449127  
0.1597134313738572 0.3444437530802607 0.5805620601082842  
0.1541521505512417 0.6572016429529799 0.5788809978884358