

Electronic and Magnetic Properties of GeS Monolayer Under Effects of Point Defects and Doping

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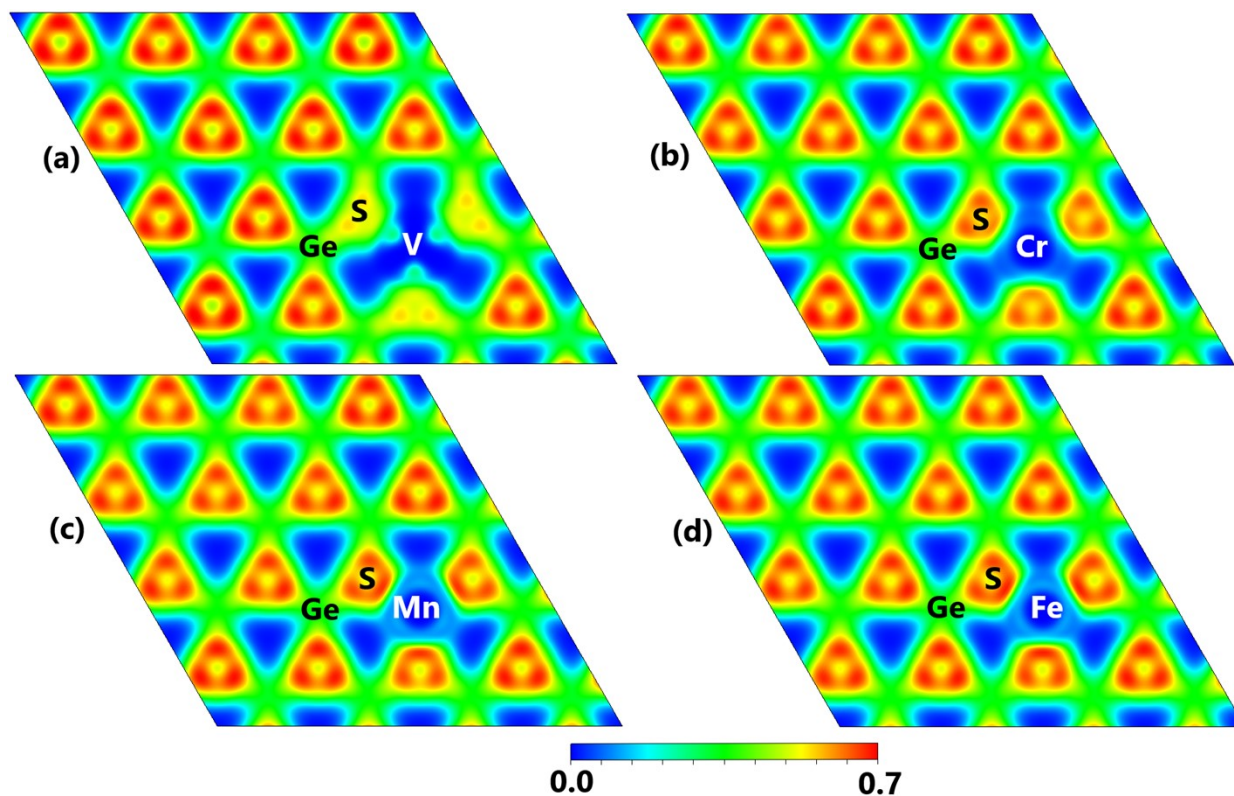


Figure S1: Electron localization function in (a) V-, (b) Cr-, (c) Mn-, and (d) Fe-doped GeS monolayer.

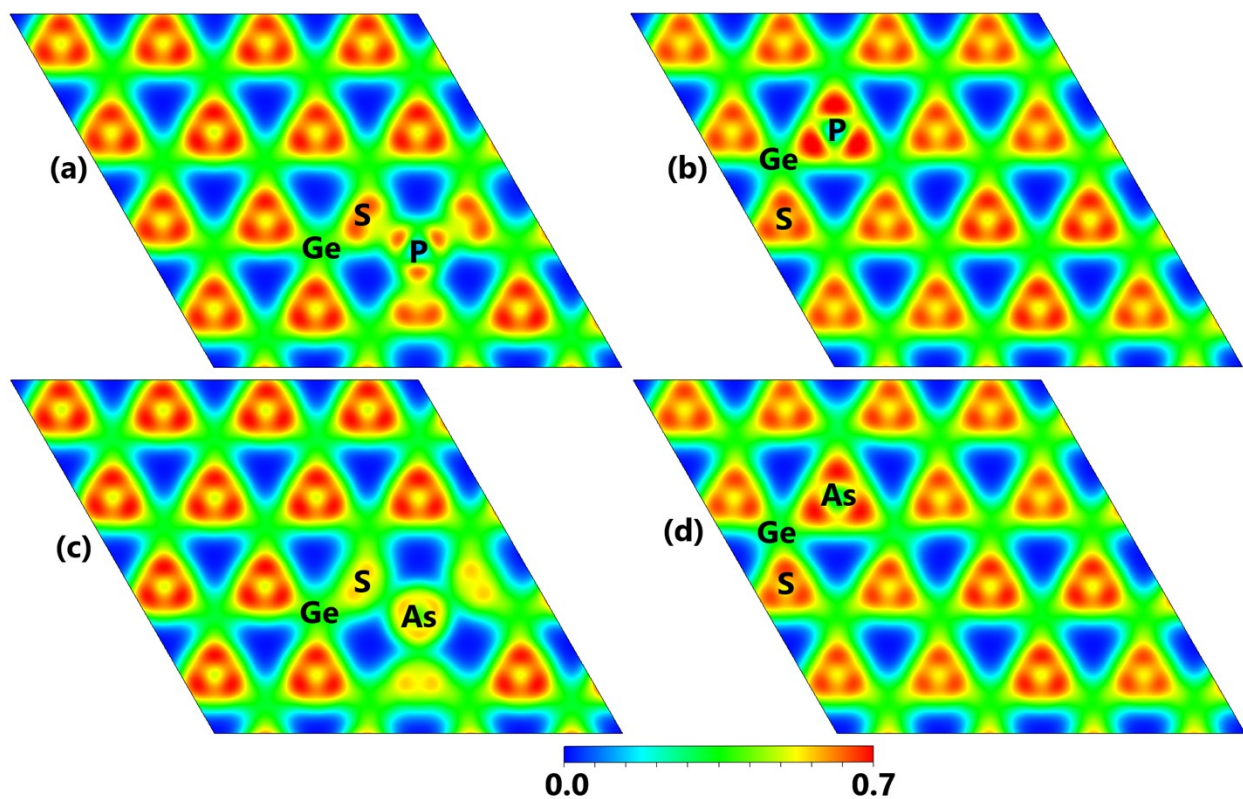


Figure S2: Electron localization function in (a) P- (at Ge site), (b) P- (at S site), (c) As- (at Ge site), and (d) As-doped (at S site) GeS monolayer.

POSCAR files of the relaxed atomic structures.

Single Ge vacancy

```

1.0000000000000000
13.9726362228000003  0.0000000000000000  0.0000000000000000
-6.9863181114000001  12.1006579268000003  0.0000000000000000
0.0000000000000000  0.0000000000000000  17.2262001038000001

```

S Ge

16 15

Direct

```

0.0846221802655018  0.1692443605309964  0.5409109098755095

```

0.0883190430849800 0.4186684585074078 0.5310263646826424
0.0883190430849800 0.6696506225775755 0.5310263646826424
0.0846221802655018 0.9153778427345037 0.5409109098755095
0.3339743254897353 0.1669871632448659 0.5514529464098281
0.3303494074224272 0.4186684585074078 0.5310263646826424
0.3333333429999996 0.6666666870000029 0.5315888512366941
0.3303494074224272 0.9116809799150255 0.5310263646826424
0.5827078156419957 0.1654156772839958 0.5409136673572742
0.5827078156419957 0.4172921843580041 0.5409136673572742
0.5813315414925921 0.6696506225775755 0.5310263646826424
0.5813315414925921 0.9116809799150255 0.5310263646826424
0.8330128217551294 0.1669871632448659 0.5514529464098281
0.8345843077159997 0.4172921843580041 0.5409136673572742
0.8330128217551294 0.6660257045102678 0.5514529464098281
0.8307556244689993 0.9153778427345037 0.5409109098755095
0.1724299664276690 0.0862149832138381 0.4662488329498681
0.1637949407278713 0.3275898804557460 0.4529133628054295
0.1678409941662242 0.5839204740831098 0.4515289353983128
0.1637949407278713 0.8362050442721242 0.4529133628054295
0.4222816751850166 0.0933071354534135 0.4683211197131190
0.4222816751850166 0.3289745317316027 0.4683211197131190
0.4160795259168897 0.5839204740831098 0.4515289353983128
0.4160795259168897 0.8321589908337708 0.4515289353983128
0.6710254982684001 0.0933071354534135 0.4683211197131190
0.6710254982684001 0.5777183248149831 0.4683211197131190
0.6724101495442562 0.8362050442721242 0.4529133628054295
0.9137850397861675 0.0862149832138381 0.4662488329498681
0.9066928875465924 0.3289745317316027 0.4683211197131190
0.9066928875465924 0.5777183248149831 0.4683211197131190
0.9137850397861675 0.8275700185723261 0.4662488329498681

Single S vacancy

1.000000000000000

13.9726362228000003 0.0000000000000000 0.0000000000000000

-6.9863181114000001 12.1006579268000003 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.2262001038000001

S Ge

15 16

Direct

0.0837028049580736 0.1674056099161400 0.5406571081605853

0.0891338634383999 0.4219573869442983 0.5370058594941602

0.0891338634383999 0.6671765144941045 0.5370058594941602

0.0837028049580736 0.9162972180419319 0.5406571081605853

0.3337443888232166 0.1668721949116065 0.5385918759041703

0.3328235155058978 0.4219573869442983 0.5370058594941602

0.3328235155058978 0.9108661595616057 0.5370058594941602

0.5827570701265675 0.1655141862531385 0.5401482531545875

0.5827570701265675 0.4172429298734326 0.5401482531545875

0.5780426130557017 0.6671765144941046 0.5370058594941602

0.5780426130557017 0.9108661595616057 0.5370058594941602

0.8331277900883884 0.1668721949116065 0.5385918759041703

0.8344857987468566 0.4172429298734326 0.5401482531545875

0.8331277900883884 0.6662556411767858 0.5385918759041703

0.8325943750838553 0.9162972180419319 0.5406571081605853

0.1656132450214935 0.0828066225107503 0.4612379900777779

0.1661038685566634 0.3322077361133303 0.4588351789410445

0.1922819273796767 0.5961409406898360 0.4663536517887756

0.1661038685566634 0.8338961164433321 0.4588351789410445

0.4175313244938649 0.0816522438440609 0.4598797280915680

0.4175313244938649 0.3358790726498032 0.4598797280915680

0.4038590593101635 0.5961409406898360 0.4663536517887756
0.4038590593101635 0.8077180576203185 0.4663536517887756
0.6641209573501994 0.0816522438440609 0.4598797280915680
0.6666666870000029 0.3333333429999996 0.4616355084047342
0.6641209573501994 0.5824686755061350 0.4598797280915680
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0.9171934004892551 0.0828066225107503 0.4612379900777779
0.9183477791559445 0.3358790726498032 0.4598797280915680
0.9183477791559445 0.5824686755061350 0.4598797280915680
0.9171934004892551 0.8343867399785015 0.4612379900777779

Ge+S divacancy

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13.9726362228000003 0.0000000000000000 0.0000000000000000
-6.9863181114000001 12.1006579268000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 17.2262001038000001

S Ge

15 15

Direct

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0.0892649651005886 0.9107350578994170 0.5388173333157635
0.3324567269163314 0.1645075644975228 0.5454234809037041
0.3271241978656492 0.4192230686391399 0.5317409010819869
0.3384179806423462 0.9123254794111831 0.5238416310691396
0.5821022350311611 0.1710407421588917 0.5420815747164709
0.5776339416587717 0.4223660583412283 0.5441073918388007
0.5807769313608602 0.6728758321343532 0.5317409010819869
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0.8289592428411036 0.4178977649688387 0.5420815747164709
0.8354924205024725 0.6675433030836638 0.5454234809037041
0.8390288410107259 0.9190299526588416 0.5418414230155950
0.1697832036545793 0.0827541841888957 0.4642926416371237
0.1686025076045624 0.3258017312343467 0.4580176616104465
0.1844829306075003 0.5784630006939764 0.4757767744780533
0.1660426132394794 0.8339573717605157 0.4491376086910844
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0.4215369993060236 0.8155170543924951 0.4757767744780533
0.6663388788958398 0.0924818985860058 0.4596871182849722
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SGe defect

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13.9726362228000003 0.0000000000000000 0.0000000000000000
-6.9863181114000001 12.1006579268000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 17.2262001038000001

S Ge

17 15

Direct

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GeS defect

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13.9726362228000003 0.0000000000000000 0.0000000000000000

-6.9863181114000001 12.1006579268000003 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.2262001038000001

S Ge

15 17

Direct

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V-doping

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-6.9863181114000001 12.1006579268000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 17.2262001038000001

S Ge V

16 15 1

Direct

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0.0831431116873770 0.9168569113126283 0.5324715903881362
0.3303019896766469 0.1651509953383217 0.5382077645921169
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0.5778412914159531 0.4221587085840469 0.5530492349684880

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0.6666666870000029 0.3333333429999996 0.5210120221692714

Cr-doping

1.0000000000000000
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-6.9863181114000001 12.1006579268000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 17.2262001038000001

S Ge Cr

16 15 1

Direct

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0.0833889421725876 0.6672100646795396 0.5383587193153880
0.0831703409084822 0.9168296820915234 0.5360237462734797
0.3323887735754562 0.1661943872877228 0.5382056103360890
0.3327899653204626 0.4161789154930440 0.5383587193153880
0.3333333429999996 0.6666666870000029 0.5390635378947801
0.3327899653204626 0.9166110808274178 0.5383587193153880
0.5818507012120059 0.1637014484240157 0.5427925516861868
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0.8338055977122727 0.6676112564245468 0.5382056103360890
0.8336593031830379 0.9168296820915234 0.5360237462734797
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0.1667265386859818 0.3334530763719671 0.4577641936708466
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0.6665469536280357 0.8332734463140133 0.4577641936708466
0.9159693582780749 0.0840306647219304 0.4570273957573531
0.9178286685569091 0.3319535968570800 0.4590783159672970

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0.9159693582780749 0.8319386555561343 0.4570273957573531
0.6666666870000029 0.3333333429999996 0.5017100416303505

Mn-doping

1.000000000000000
13.9726362228000003 0.0000000000000000 0.0000000000000000
-6.9863181114000001 12.1006579268000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 17.2262001038000001

S Ge Mn

16 15 1

Direct

0.0830585730351263 0.1661171460702455 0.5368718655718768
0.0824738970358067 0.4164098989928339 0.5400527469214852
0.0824738970358067 0.6660640360429761 0.5400527469214852
0.0830585730351263 0.9169414499648790 0.5368718655718768
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0.5841979240040359 0.4158020759959642 0.5384538789725348
0.5835901010071666 0.6660640360429761 0.5400527469214852
0.5835901010071666 0.9175261259641984 0.5400527469214852
0.8336409433536952 0.1663590416463000 0.5377278540060940
0.8316040909919198 0.4158020759959642 0.5384538789725348
0.8336409433536952 0.6672819477073991 0.5377278540060940
0.8338828389297497 0.9169414499648790 0.5368718655718768
0.1675808076182308 0.0837904038091190 0.4574361299792640
0.1671593756127036 0.3343187502254106 0.4598111177769813

0.1668847988269519 0.5834423764134742 0.4613881383660166
0.1671593756127036 0.8328406093872921 0.4598111177769813
0.4129726727288064 0.0811346787243337 0.4582861083192670
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0.6656812797745923 0.8328406093872921 0.4598111177769813
0.9162096191908866 0.0837904038091190 0.4574361299792640
0.9188653442756718 0.3318379860044723 0.4582861083192670
0.9188653442756718 0.5870273272711936 0.4582861083192670
0.9162096191908866 0.8324191773817643 0.4574361299792640
0.6666666870000029 0.3333333429999996 0.4939390647729999

Fe-doping

1.0000000000000000
13.9726362228000003 0.0000000000000000 0.0000000000000000
-6.9863181114000001 12.1006579268000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 17.2262001038000001

S Ge Fe

16 15 1

Direct

0.0832445302957577 0.1664890605915083 0.5393627892088202
0.0816136422271535 0.4167301361106068 0.5395365357495417
0.0816136422271535 0.6648835441165505 0.5395365357495417
0.0832445302957577 0.9167554927042475 0.5393627892088202
0.3335375863995838 0.1667687936997901 0.5380898210775176
0.3351164858834524 0.4167301361106068 0.5395365357495417
0.3333333429999996 0.6666666870000029 0.5397127924377242

0.3351164858834524 0.9183863807728516 0.5395365357495417
0.5859704167942162 0.1719408795884362 0.5375277214063851
0.5859704167942162 0.4140295832057838 0.5375277214063851
0.5832698638893933 0.6648835441165505 0.5395365357495417
0.5832698638893933 0.9183863807728516 0.5395365357495417
0.8332311913002051 0.1667687936997901 0.5380898210775176
0.8280591054115590 0.4140295832057838 0.5375277214063851
0.8332311913002051 0.6664624436004186 0.5380898210775176
0.8335109244084868 0.9167554927042475 0.5393627892088202
0.1664972974599195 0.0832486487299633 0.4596288351459921
0.1666249981596253 0.3332499953192540 0.4607513625717223
0.1664885557830123 0.5832442548915040 0.4604768533748120
0.1666249981596253 0.8333749868403704 0.4607513625717223
0.4140118270502181 0.0828120357412248 0.4575702798472610
0.4140118270502181 0.3311997833089925 0.4575702798472610
0.4167557451084958 0.5832442548915040 0.4604768533748120
0.4167557451084958 0.8335114292169831 0.4604768533748120
0.6688002466910102 0.0828120357412248 0.4575702798472610
0.6688002466910102 0.5859881729497820 0.4575702798472610
0.6667500346807484 0.8333749868403704 0.4607513625717223
0.9167513742700423 0.0832486487299633 0.4596288351459921
0.9171879872587806 0.3311997833089925 0.4575702798472610
0.9171879872587806 0.5859881729497820 0.4575702798472610
0.9167513742700423 0.8335026875400755 0.4596288351459921
0.6666666870000029 0.3333333429999996 0.4901346456256383

P at Ge

1.00000000000000

13.9726362228000003 0.0000000000000000 0.0000000000000000

-6.9863181114000001 12.1006579268000003 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.2262001038000001

S Ge P

16 15 1

Direct

0.0831483178867909 0.1662966357735746 0.5382777207151580
0.0815057029527960 0.4157307940187202 0.5377114901124178
0.0815057029527960 0.6657749469340790 0.5377114901124178
0.0831483178867909 0.9168517051132151 0.5382777207151580
0.3322310226794699 0.1661155118397332 0.5368678510217709
0.3342250830659237 0.4157307940187202 0.5377114901124178
0.3333333429999996 0.6666666870000029 0.5352141169655541
0.3342250830659237 0.9184943200472093 0.5377114901124178
0.5852462654722751 0.1704925769445539 0.5466796293145280
0.5852462654722751 0.4147537345277251 0.5466796293145280
0.5842692059812796 0.6657749469340790 0.5377114901124178
0.5842692059812796 0.9184943200472093 0.5377114901124178
0.8338844731602619 0.1661155118397332 0.5368678510217709
0.8295074080554415 0.4147537345277251 0.5466796293145280
0.8338844731602619 0.6677690073205328 0.5368678510217709
0.8337033492264210 0.9168517051132151 0.5382777207151580
0.1647569672343182 0.0823784836171627 0.4578633773553338
0.1660298463358665 0.3320596916717365 0.4591666094810476
0.1640756140523898 0.5820377840261929 0.4579931647735764
0.1660298463358665 0.8339701386641286 0.4591666094810476
0.4215240222727046 0.0863782357898390 0.4596316643991089
0.4215240222727046 0.3351457784828649 0.4596316643991089
0.4179622159738072 0.5820377840261929 0.4579931647735764
0.4179622159738072 0.8359243709476057 0.4579931647735764
0.6648542515171380 0.0863782357898390 0.4596316643991089
0.6648542515171380 0.5784759777272953 0.4596316643991089

0.6679403383282662 0.8339701386641286 0.4591666094810476
0.9176215393828427 0.0823784836171627 0.4578633773553338
0.9136217872101662 0.3351457784828649 0.4596316643991089
0.9136217872101662 0.5784759777272953 0.4596316643991089
0.9176215393828427 0.8352430177656768 0.4578633773553338
0.6666666870000029 0.3333333429999996 0.4901823779809656

P at S

1.0000000000000000
13.9726362228000003 0.0000000000000000 0.0000000000000000
-6.9863181114000001 12.1006579268000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 17.2262001038000001

S Ge P

15 16 1

Direct

0.0835172987827787 0.1670345975655504 0.5417641421327597
0.0827303151216185 0.4155329824892960 0.5411702207576401
0.0827303151216185 0.6671973706323256 0.5411702207576401
0.0835172987827787 0.9164827242172267 0.5417641421327597
0.3333823748915710 0.1666911879457837 0.5414275734454762
0.3328026593676771 0.4155329824892960 0.5411702207576401
0.3328026593676771 0.9172697078783870 0.5411702207576401
0.5833652816618005 0.1667306093235969 0.5379245233516041
0.5833652816618005 0.4166347183381999 0.5379245233516041
0.5844670175107040 0.6671973706323256 0.5411702207576401
0.5844670175107040 0.9172697078783870 0.5411702207576401
0.8333087970542110 0.1666911879457837 0.5414275734454762
0.8332693756763982 0.4166347183381999 0.5379245233516041
0.8333087970542110 0.6666176551084312 0.5414275734454762
0.8329653874344449 0.9164827242172267 0.5417641421327597

0.1669028406175476 0.0834514203087773 0.4627746179083465
 0.1662964938365449 0.3325929866730932 0.4619772044039185
 0.1529809862687873 0.5764904701343950 0.4582764484448452
 0.1662964938365449 0.8337034911634499 0.4619772044039185
 0.4144999549407732 0.0822296870263456 0.4609734068751238
 0.4144999549407732 0.3322702599144269 0.4609734068751238
 0.4235095298656047 0.5764904701343950 0.4582764484448452
 0.4235095298656047 0.8470189987312079 0.4582764484448452
 0.6677297700855757 0.0822296870263456 0.4609734068751238
 0.6666666870000029 0.3333333429999996 0.4584288898166274
 0.6677297700855757 0.5855000450592267 0.4609734068751238
 0.6674070433269091 0.8337034911634499 0.4619772044039185
 0.9165486026912278 0.0834514203087773 0.4627746179083465
 0.9177703359736598 0.3322702599144269 0.4609734068751238
 0.9177703359736598 0.5855000450592267 0.4609734068751238
 0.9165486026912278 0.8330971443824478 0.4627746179083465
 0.3333333429999996 0.6666666870000029 0.5162762953258628

As at Ge

1.000000000000000
 13.9726362228000003 0.0000000000000000 0.0000000000000000
 -6.9863181114000001 12.1006579268000003 0.0000000000000000
 0.0000000000000000 0.0000000000000000 17.2262001038000001

S Ge As

16 15 1

Direct

0.0832707998474648 0.1665415996949153 0.5361505628244440
 0.0847515695508262 0.4160765859195911 0.5357307650249804
 0.0847515695508262 0.6686750216312379 0.5357307650249804
 0.0832707998474648 0.9167292231525409 0.5361505628244440

0.3321588748328408 0.1660794379164187 0.5367005944177233
0.3313250083687641 0.4160765859195911 0.5357307650249804
0.3333333429999996 0.6666666870000029 0.5362784334267704
0.3313250083687641 0.9152484534491794 0.5357307650249804
0.5768969251833498 0.1537938963667104 0.5527528572524574
0.5768969251833498 0.4231030748166504 0.5527528572524574
0.5839234140804090 0.6686750216312379 0.5357307650249804
0.5839234140804090 0.9152484534491794 0.5357307650249804
0.8339205470835764 0.1660794379164187 0.5367005944177233
0.8462060886332851 0.4231030748166504 0.5527528572524574
0.8339205470835764 0.6678411551671620 0.5367005944177233
0.8334583853050795 0.9167292231525409 0.5361505628244440
0.1658035821900170 0.0829017910950120 0.4567604606483979
0.1660796496301106 0.3321592982602175 0.4560106733581211
0.1668231159157201 0.5834115349578619 0.4570003307843499
0.1660796496301106 0.8339203353698847 0.4560106733581211
0.4233391166375885 0.0866102345609482 0.4609541934495899
0.4233391166375885 0.3367288740766467 0.4609541934495899
0.4165884650421383 0.5834115349578619 0.4570003307843499
0.4165884650421383 0.8331768690842750 0.4570003307843499
0.6632711559233558 0.0866102345609482 0.4609541934495899
0.6632711559233558 0.5766608833624118 0.4609541934495899
0.6678407317397846 0.8339203353698847 0.4560106733581211
0.9170982319049936 0.0829017910950120 0.4567604606483979
0.9133897884390570 0.3367288740766467 0.4609541934495899
0.9133897884390570 0.5766608833624118 0.4609541934495899
0.9170982319049936 0.8341964028099780 0.4567604606483979
0.6666666870000029 0.3333333429999996 0.4974858578692628

As at S

1.0000000000000000

13.9726362228000003 0.0000000000000000 0.0000000000000000

-6.9863181114000001 12.1006579268000003 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.2262001038000001

S Ge As

15 16 1

Direct

0.0835285884931615 0.1670571769863160 0.5412221471687370

0.0814315191801853 0.4145895911523482 0.5413049973899811

0.0814315191801853 0.6668419660278405 0.5413049973899811

0.0835285884931615 0.9164714345068439 0.5412221471687370

0.3329508932132786 0.1664754471066411 0.5420332094630339

0.3331580639721621 0.4145895911523482 0.5413049973899811

0.3331580639721621 0.9185685038198200 0.5413049973899811

0.5834206781337449 0.1668414022675009 0.5382363893032989

0.5834206781337449 0.4165793218662550 0.5382363893032989

0.5854104088476522 0.6668419660278405 0.5413049973899811

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0.8335245378933538 0.1664754471066411 0.5420332094630339

0.8331585827324942 0.4165793218662550 0.5382363893032989

0.8335245378933538 0.6670491367867241 0.5420332094630339

0.8329428080136794 0.9164714345068439 0.5412221471687370

0.1674420877849905 0.0837210438924988 0.4624678018591973

0.1665391598348328 0.3330783186696690 0.4620524024082090

0.1463445685725106 0.5731722612862533 0.4566480073810973

0.1665391598348328 0.8334608251651624 0.4620524024082090

0.4144833529117477 0.0829618692930777 0.4612919151988792

0.4144833529117477 0.3315214756186698 0.4612919151988792

0.4268277387137466 0.5731722612862533 0.4566480073810973

0.4268277387137466 0.8536554164274845 0.4566480073810973

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0.6684785543813326 0.5855166470882524 0.4612919151988792
0.6669217113303333 0.8334608251651624 0.4620524024082090
0.9162789791075067 0.0837210438924988 0.4624678018591973
0.9170381537069282 0.3315214756186698 0.4612919151988792
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