

Supporting Information

Structural morphologies of high-pressure polymorphs of strontium hydrides

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I. Structural information

1. $P6_3/mmc$ structure of SrH_2 at 50 GPa

```
POSCAR FORMAT
1.0
3.6040809637023004 0.0000000000000000 0.0000000000000000
-1.8020404818511502 3.1212256718620930 0.0000000000000000
0.0000000000000000 0.0000000000000000 4.5131562969550165
H Sr
4 2
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.5000000000000000
0.3333333333333333 0.6666666666666667 0.7500000000000000
0.6666666666666667 0.3333333333333333 0.2500000000000000
0.3333333333333333 0.6666666666666667 0.2500000000000000
0.6666666666666667 0.3333333333333333 0.7500000000000000
```

2. $P6/mmm$ structure of SrH_2 at 150 GPa

```
POSCAR FORMAT
1.0
2.8011645733524384 0.0000000000000000 0.0000000000000000
-1.4005822866762192 2.4258796807042105 0.0000000000000000
0.0000000000000000 0.0000000000000000 2.5489670854399149
H Sr
2 1
Direct
0.3333333333333333 0.6666666666666667 0.5000000000000000
0.6666666666666667 0.3333333333333333 0.5000000000000000
0.0000000000000000 0.0000000000000000 0.0000000000000000
```

3. $I4/mmm$ structure of SrH_4 at 50 GPa

```
POSCAR FORMAT
1.0
3.2988023818914578 0.0000000000000000 0.0000000000000000
0.0000000000000000 3.2988023818914578 0.0000000000000000
0.0000000000000000 0.0000000000000000 5.6436935495784333
H Sr
8 2
Direct
0.0000000000000000 0.0000000000000000 0.9298214286369852
0.0000000000000000 0.0000000000000000 0.0701785713630147
0.5000000000000000 0.0000000000000000 0.2500000000000000
0.0000000000000000 0.5000000000000000 0.2500000000000000
0.5000000000000000 0.5000000000000000 0.4298214286369852
0.5000000000000000 0.5000000000000000 0.5701785713630148
0.0000000000000000 0.5000000000000000 0.7500000000000000
0.5000000000000000 0.0000000000000000 0.7500000000000000
0.5000000000000000 0.5000000000000000 0.0000000000000000
0.0000000000000000 0.5000000000000000 0.5000000000000000
```

4. $Cmcm$ structure of SrH_4 at 150 GPa

```
POSCAR FORMAT
1.0
2.7686732849525133 0.0000000000000000 0.0000000000000000
0.0000000000000000 6.5773053558312151 0.0000000000000000
0.0000000000000000 0.0000000000000000 4.6779524550073850
H Sr
16 4
Direct
0.0000000000000000 0.7894439066756838 0.1627852833508430
0.5000000000000000 0.8731128602138252 0.4202505545334611
0.0000000000000000 0.2105560933243163 0.6627852833508430
0.5000000000000000 0.1268871397861749 0.9202505545334611
0.0000000000000000 0.7894439066756838 0.3372147166491570
0.5000000000000000 0.8731128602138252 0.0797494454665389
0.0000000000000000 0.2105560933243163 0.8372147166491570
0.5000000000000000 0.1268871397861749 0.5797494454665389
0.0000000000000000 0.2894439066756838 0.1627852833508430
0.0000000000000000 0.3731128602138251 0.4202505545334611
0.5000000000000000 0.7105560933243162 0.6627852833508430
0.0000000000000000 0.6268871397861748 0.9202505545334611
0.5000000000000000 0.2894439066756838 0.3372147166491570
0.0000000000000000 0.3731128602138251 0.0797494454665389
0.5000000000000000 0.7105560933243162 0.8372147166491570
0.0000000000000000 0.6268871397861748 0.5797494454665389
0.0000000000000000 0.9121306864066739 0.7500000000000000
0.0000000000000000 0.0878693135933260 0.2500000000000000
0.5000000000000000 0.4121306864066739 0.7500000000000000
0.5000000000000000 0.5878693135933261 0.2500000000000000
```

5. $C2/c$ structure of SrH_6 at 50 GPa

```
POSCAR FORMAT
1.0
3.3217784225418678 -0.0000000000000000 0.5259639979329169
0.0000000000000000 -0.0000000000000000 -3.8325278091763786
1.6608892112709339 5.5704694010016329 0.2629819989664585
H Sr
12 2
Direct
0.0517550582510135 0.2815123672690953 0.6839419538093476
0.7356970120603611 0.7815123672690953 0.3160580461906524
0.9183399435631054 0.4499485820090264 0.9682815221542558
0.1133785342826388 0.0500514179909736 0.9682815221542558
0.0816600564368946 0.5500514179909737 0.0317184778457442
0.2560901919555997 0.7500000000000000 0.4878196160888006
0.4464333729285122 0.7500000000000000 0.1071332541429756
0.7439098080444003 0.2500000000000000 0.5121803839111994
```

0.8866214657173612 0.9499485820090263 0.0317184778457442
0.2643029879396389 0.2184876327309047 0.6839419538093476
0.5535666270714878 0.2500000000000000 0.8928667458570243
0.9482449417489865 0.7184876327309047 0.3160580461906524
0.3614791622010887 0.2500000000000000 0.2770416755978227
0.6385208377989113 0.7500000000000000 0.7229583244021773

0.9433495095576876 0.3284698369059784 0.8146859134377744
0.9559765094503316 0.6161205491823031 0.8526987044593966
0.6715301630940216 0.6148796726517092 0.8146859134377744
0.0440234905496683 0.6601440397319713 0.1473012955406034
0.3284698369059784 0.9433495095576876 0.1853140865622256
0.6161205491823031 0.9559765094503316 0.1473012955406034
0.6148796726517092 0.6715301630940216 0.1853140865622256
0.3398559602680286 0.3838794508176969 0.1473012955406034
0.0566504904423125 0.3851203273482908 0.1853140865622256
0.2895410794303041 0.0000000000000000 0.5000000000000000
0.0000000000000000 0.2895410794303041 0.5000000000000000
0.7104589205696958 0.7104589205696958 0.5000000000000000
0.2749020839345468 0.2749020839345468 0.5000000000000000
0.7250979160654532 0.0000000000000000 0.5000000000000000
0.0000000000000000 0.7250979160654532 0.5000000000000000
0.3333333333333333 0.6666666666666667 0.6679793566182153
0.6666666666666667 0.3333333333333333 0.3320206433817847
0.0000000000000000 0.0000000000000000 0.0000000000000000

6. $P\bar{3}$ structure of SrH_6 at 150 GPa

POSCAR FORMAT

H Sr

1.0

5.3658169499267201 0.0000000000000000 0.0000000000000000
-2.6829084749633600 4.6469337906936730 0.0000000000000000
0.0000000000000000 0.0000000000000000 2.9995097207669144

H Sr

18 3

Direct

0.7212740451617539 0.0086892128797895 0.0330969678397537
0.0602883323441337 0.6632099009347907 0.6464629188982514
0.9538414619390329 0.6304985022334246 0.3041329644319504
0.9913107871202105 0.7125848322819643 0.0330969678397537
0.3367900990652093 0.3970784314093431 0.6464629188982514
0.3695014977665754 0.3233429597056082 0.3041329644319504
0.2874151677180356 0.2787259548382461 0.0330969678397537
0.6029215685906569 0.9397116676558662 0.6464629188982514
0.6766570402943918 0.0461585380609672 0.3041329644319504
0.2787259548382461 0.9913107871202105 0.9669030321602463
0.9397116676558662 0.3367900990652093 0.3535370811017486
0.0461585380609672 0.3695014977665754 0.6958670355680496
0.0086892128797895 0.2874151677180356 0.9669030321602463
0.6632099009347907 0.6029215685906569 0.3535370811017486
0.6304985022334246 0.6766570402943918 0.6958670355680496
0.7125848322819643 0.7212740451617539 0.9669030321602463
0.3970784314093431 0.0602883323441337 0.3535370811017486
0.3233429597056082 0.9538414619390329 0.6958670355680496
0.3333333333333333 0.6666666666666667 0.1664880721487307
0.6666666666666667 0.3333333333333333 0.8335119278512693
0.0000000000000000 0.0000000000000000 0.5000000000000000

7. $P321$ structure of SrH_6 at 200 GPa

POSCAR FORMAT

1.0

5.2329763528329289 0.0000000000000000 0.0000000000000000
-2.6164881764164645 4.5318904589565561 0.0000000000000000
0.0000000000000000 0.0000000000000000 2.8668266786331889

H Sr

18 3

Direct

0.3838794508176969 0.3398559602680286 0.8526987044593966
0.3851203273482908 0.0566504904423125 0.8146859134377744
0.6601440397319713 0.0440234905496683 0.8526987044593966

8. $R\bar{3}m$ structure of SrH_6 at 300 GPa

POSCAR FORMAT

1.0

2.5595334951422015 -1.4777473524202138 0.9267824785169128
0.0000000000000000 2.9554947048404276 0.9267824785169128
-2.5595334951422015 -1.4777473524202138 0.9267824785169128

H Sr

6 1

Direct

0.7811607503129375 0.2188392496870625 0.5000000000000000
0.5000000000000000 0.7811607503129375 0.2188392496870625
0.2188392496870625 0.5000000000000000 0.7811607503129375
0.2188392496870625 0.7811607503129375 0.5000000000000000
0.5000000000000000 0.2188392496870625 0.7811607503129375
0.7811607503129375 0.5000000000000000 0.2188392496870625
0.0000000000000000 0.0000000000000000 0.0000000000000000

9. $Cmc2_1$ structure of SrH_8 at 50 GPa

POSCAR FORMAT

1.0

3.9552883623960846 0.0000000000000000 0.0000000000000000
0.0000000000000000 6.5565050346057587 0.0000000000000000
0.0000000000000000 0.0000000000000000 6.2702954318134383

H Sr

32 4

Direct

0.3089769318710255 0.8807014251431242 0.5213697025107490
0.7854229309316328 0.0271938839343499 0.9725832571090852
0.6910230681289745 0.1192985748568758 0.0213697025107490
0.2145770690683672 0.9728061160656500 0.4725832571090852
0.3089769318710255 0.1192985748568758 0.0213697025107490
0.7854229309316328 0.9728061160656500 0.4725832571090852

0.6910230681289745 0.8807014251431242 0.5213697025107490
0.2145770690683672 0.0271938839343499 0.9725832571090852
0.0000000000000000 0.9441942515168128 0.1767499056793572
0.0000000000000000 0.0067589070483687 0.2836415149211891
0.0000000000000000 0.1682543103671878 0.5062943401655433
0.0000000000000000 0.0558057484831872 0.6767499056793572
0.0000000000000000 0.9932410929516313 0.7836415149211891
0.0000000000000000 0.8317456896328123 0.0062943401655433
0.0000000000000000 0.6643827937062465 0.3158156901380649
0.0000000000000000 0.3356172062937535 0.8158156901380649
0.8089769318710255 0.3807014251431242 0.5213697025107490
0.2854229309316328 0.5271938839343500 0.9725832571090852
0.1910230681289745 0.6192985748568758 0.0213697025107490
0.7145770690683672 0.4728061160656501 0.4725832571090852
0.8089769318710255 0.6192985748568758 0.0213697025107490
0.2854229309316328 0.4728061160656501 0.4725832571090852
0.1910230681289745 0.3807014251431242 0.5213697025107490
0.7145770690683672 0.5271938839343500 0.9725832571090852
0.5000000000000000 0.4441942515168129 0.1767499056793572
0.5000000000000000 0.5067589070483687 0.2836415149211891
0.5000000000000000 0.6682543103671877 0.5062943401655433
0.5000000000000000 0.5558057484831872 0.6767499056793572
0.5000000000000000 0.4932410929516313 0.7836415149211891
0.5000000000000000 0.3317456896328123 0.0062943401655433
0.5000000000000000 0.1643827937062465 0.3158156901380649
0.5000000000000000 0.8356172062937535 0.8158156901380649
0.0000000000000000 0.6722983567095266 0.6956807854218380
0.0000000000000000 0.3277016432904733 0.1956807854218380
0.5000000000000000 0.1722983567095267 0.6956807854218380
0.5000000000000000 0.8277016432904734 0.1956807854218380

10. $P2_1/c$ structure of SrH_8 at 150 GPa

POSCAR FORMAT

1.0

3.4732235165897904 0.0000000000000000 0.2289609751046975
0.0000000000000000 5.9924444975902960 0.0000000000000000
0.0000000000000000 0.0000000000000000 2.754357728564066

H Sr

16 2

Direct

0.4998500701199760 0.3343241673493935 0.4746934398274831
0.7834376709079507 0.7629836985845913 0.9231252419616069
0.5138269409246163 0.4648463242173619 0.1186177608729224
0.1679067560029281 0.7818961352492906 0.1630191902307558
0.0001499298800240 0.8343241673493935 0.5253065601725169
0.7165623290920493 0.2629836985845913 0.0768747580383931
0.9861730590753837 0.9648463242173619 0.8813822391270776
0.3320932439970719 0.2818961352492906 0.8369808097692442
0.5001499298800240 0.6656758326506065 0.5253065601725169
0.2165623290920493 0.2370163014154087 0.0768747580383931
0.4861730590753837 0.5351536757826381 0.8813822391270776
0.8320932439970719 0.2181038647507094 0.8369808097692442

0.9998500701199760 0.1656758326506065 0.4746934398274831
0.2834376709079507 0.7370163014154087 0.9231252419616069
0.0138269409246163 0.0351536757826381 0.1186177608729224
0.6679067560029281 0.7181038647507094 0.1630191902307558
0.5000000000000000 0.0000000000000000 0.5000000000000000
0.0000000000000000 0.5000000000000000 0.5000000000000000

11. $P2_1/m$ structure of SrH_{10} at 50 GPa

POSCAR FORMAT

1.0

4.6604499220251032 0.0000000000000000 0.0156732334987082
0.0000000000000000 5.9711714173391579 0.0000000000000000
-0.010338952758415 0.0000000000000000 3.3295204631718596

H Sr

20 2

Direct

0.3788169341926005 0.3172972236160890 0.2501349024686583
0.6211830658073995 0.8172972236160889 0.7498650975313413
0.9271201699695188 0.4409928067332496 0.2499725677163797
0.0728798300304814 0.9409928067332494 0.7500274322836203
0.8266925055729040 0.8138183656932789 0.2497843403833983
0.1733074944270957 0.3138183656932793 0.7502156596166015
0.3581253024811623 0.9865651461389255 0.7500154093706356
0.6418746975188376 0.4865651461389258 0.2499845906293644
0.1733074944270957 0.1861816343067206 0.7502156596166015
0.8266925055729040 0.6861816343067211 0.2497843403833983
0.3788169341926005 0.1827027763839112 0.2501349024686583
0.6211830658073995 0.6827027763839111 0.7498650975313413
0.0842523510799164 0.3935908765479342 0.2501841226156671
0.9157476489200836 0.8935908765479341 0.7498158773843326
0.6418746975188376 0.0134348538610742 0.2499845906293644
0.3581253024811623 0.5134348538610745 0.7500154093706356
0.0728798300304814 0.5590071932667506 0.7500274322836203
0.9271201699695188 0.0590071932667506 0.2499725677163797
0.9157476489200836 0.6064091234520659 0.7498158773843326
0.0842523510799164 0.1064091234520657 0.2501841226156671
0.6809195462920128 0.2500000000000000 0.7499587696357506
0.3190804537079872 0.7500000000000000 0.2500412303642494

12. $P2/c$ structure of SrH_{10} at 150 GPa

POSCAR FORMAT

1.0

3.3455364672474337 0.0000000000000000 -0.0011974026124724
0.0000000000000000 3.7699941763425233 0.0000000000000000
0.0000000000000000 0.0000000000000000 5.0946366348419154

H Sr

20 2

Direct

0.7500230046558185 0.2508028960109246 0.9612872053432688
0.2500230046558185 0.7491971039890755 0.4612872053432688
0.0159326308155118 0.2495849397599327 0.3315352264472765

0.5159326308155118 0.7504150602400672 0.8315352264472765
 0.9831456331582743 0.7504363288245978 0.8315490897625172
 0.4831456331582743 0.2495636711754022 0.3315490897625172
 0.2498016279246337 0.5038675350045867 0.0892564305807554
 0.7498016279246337 0.4961324649954132 0.5892564305807554
 0.7501983720753663 0.4961324649954132 0.9107435694192446
 0.2501983720753663 0.5038675350045867 0.4107435694192446
 0.5168543668417257 0.7504363288245978 0.6684509102374828
 0.0168543668417257 0.2495636711754022 0.1684509102374828
 0.2502262097593102 0.9956721297462874 0.4109494219950287
 0.7502262097593102 0.0043278702537126 0.9109494219950287
 0.7497737902406898 0.0043278702537126 0.5890505780049713
 0.2497737902406898 0.9956721297462874 0.0890505780049713
 0.9840673691844882 0.7504150602400672 0.6684647735527235
 0.4840673691844882 0.2495849397599327 0.1684647735527235
 0.7499769953441815 0.2508028960109246 0.5387127946567312
 0.2499769953441815 0.7491971039890755 0.0387127946567312
 0.7500000000000000 0.7499384229536448 0.2500000000000000
 0.2500000000000000 0.2500615770463552 0.7500000000000000

12. $R\bar{3}m$ structure of SrH₁₀ at 300 GPa

POSCAR FORMAT

1.0

1.6875400304939401 -0.9743016908739456 2.5618411825545899
 0.0000000000000000 1.9486033817478912 2.5618411825545899
 -1.6875400304939401 -0.9743016908739456 2.5618411825545899

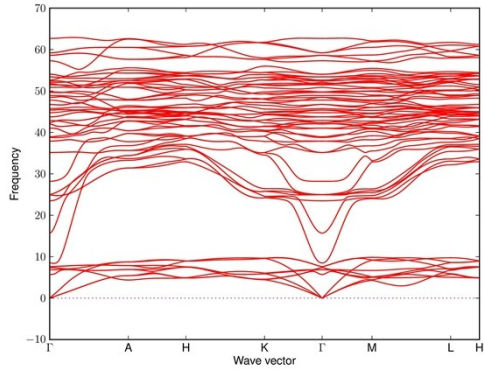
H Sr

10 1

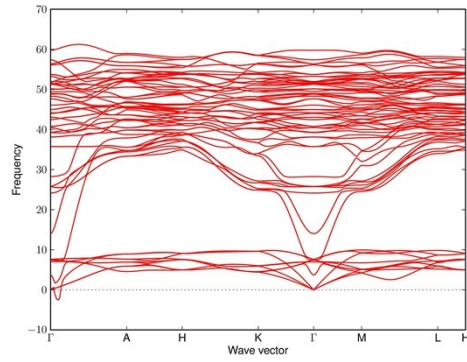
Direct

0.0976773820283206 0.0976773820283206 0.0976773820283206
 0.3811274739358967 0.8947680931077198 0.8947680931077198
 0.8947680931077198 0.8947680931077198 0.3811274739358967
 0.2582915112288267 0.2582915112288267 0.2582915112288267
 0.6188725260641033 0.1052319068922802 0.1052319068922802
 0.8947680931077198 0.3811274739358967 0.8947680931077198
 0.7417084887711733 0.7417084887711733 0.7417084887711733
 0.1052319068922802 0.1052319068922802 0.6188725260641033
 0.1052319068922802 0.6188725260641033 0.1052319068922802
 0.9023226179716793 0.9023226179716793 0.9023226179716793
 0.5000000000000000 0.5000000000000000 0.5000000000000000

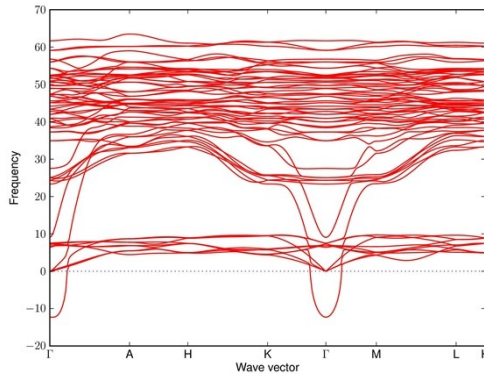
II. Phonon spectrum



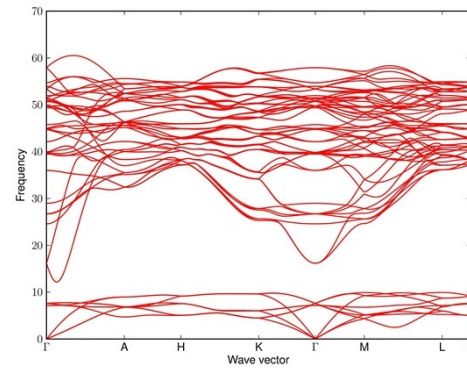
$P\bar{3}$ structure of SrH₆ at 195 GPa



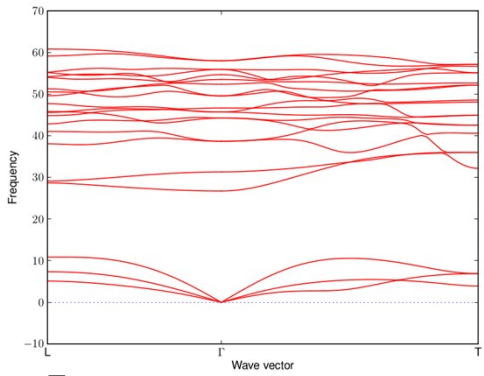
$P\bar{3}$ structure of SrH₆ at 200 GPa



P321 structure of SrH₆ at 190 GPa



P321 structure of SrH₆ at 200 GPa



$R\bar{3}m$ structure of SrH₆ at 250 GPa