

Electronic supplementary information (ESI)

**Investigation of strain behavior and carrier mobility on organic-inorganic hybrid perovskite :
(C₄H₉NH₃)₂GeI₄ and (C₄H₉NH₃)₂SnI₄**

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1 The monolayer (C₄H₉NH₃)₂GeI₄ and (C₄H₉NH₃)₂SnI₄ under biaxial strain with organic molecules removed from the structure.

2 Ab initio molecular dynamics (AIMD) simulations for monolayer (C₄H₉NH₃)₂GeI₄ and (C₄H₉NH₃)₂SnI₄.

3 Electronic band structure for monolayer (C₄H₉NH₃)₂GeI₄ and (C₄H₉NH₃)₂SnI₄ based on PBE-SOC.

4 POSCAR file with space group C222 (No. 21) and PBCA (No. 61) for bulk (C₄H₉NH₃)₂GeI₄ and (C₄H₉NH₃)₂SnI₄

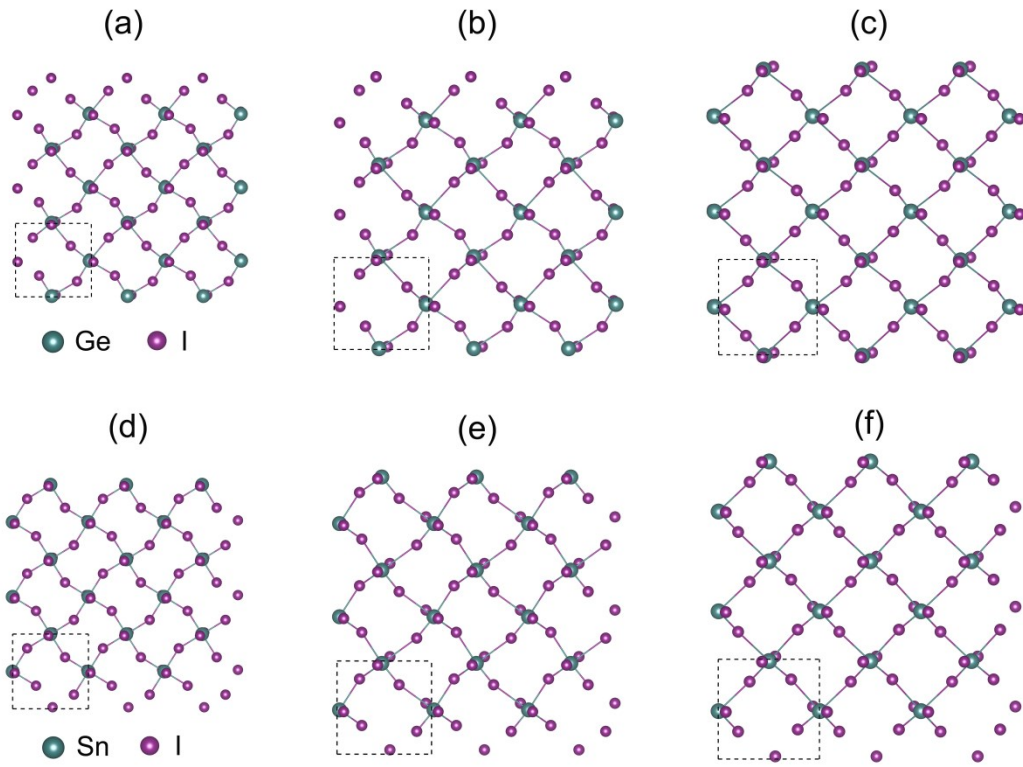


Fig. S1. The monolayer $(\text{C}_4\text{H}_9\text{NH}_3)_2\text{GeI}_4$ and $(\text{C}_4\text{H}_9\text{NH}_3)_2\text{SnI}_4$ under biaxial strain with organic molecules removed from the structure. (a), (b) and (c) denotes the atomic structure of $(\text{C}_4\text{H}_9\text{NH}_3)_2\text{GeI}_4$ at the biaxial strain of $\epsilon = 0$, $\epsilon = 13\%$, and $\epsilon = 14\%$. (d), (e) and (f) denotes the atomic structure of $(\text{C}_4\text{H}_9\text{NH}_3)_2\text{SnI}_4$ at the biaxial strain of $\epsilon = 0$, $\epsilon = 15\%$ and $\epsilon = 16\%$.

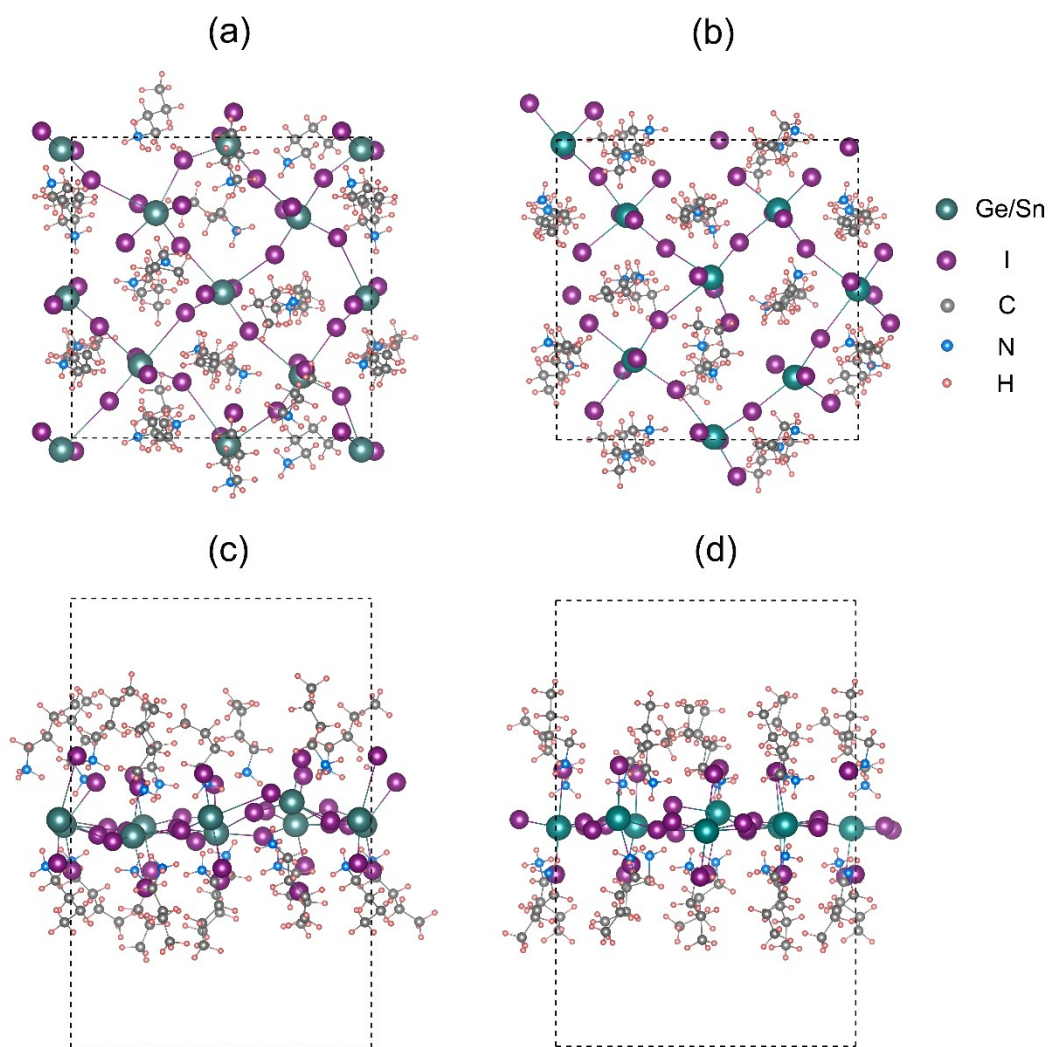


Fig. S2. Ab initio molecular dynamics (AIMD) simulations in 2×2 supercell with the NVT ensemble. At 300 K, the system at biaxial strain of $\epsilon=8\%$ runs 3000 steps with a step length of 0.5 fs. (a), (c) top and side views for $(\text{C}_4\text{H}_9\text{NH}_3)_2\text{GeI}_4$; (b), (d) for $(\text{C}_4\text{H}_9\text{NH}_3)_2\text{SnI}_4$.

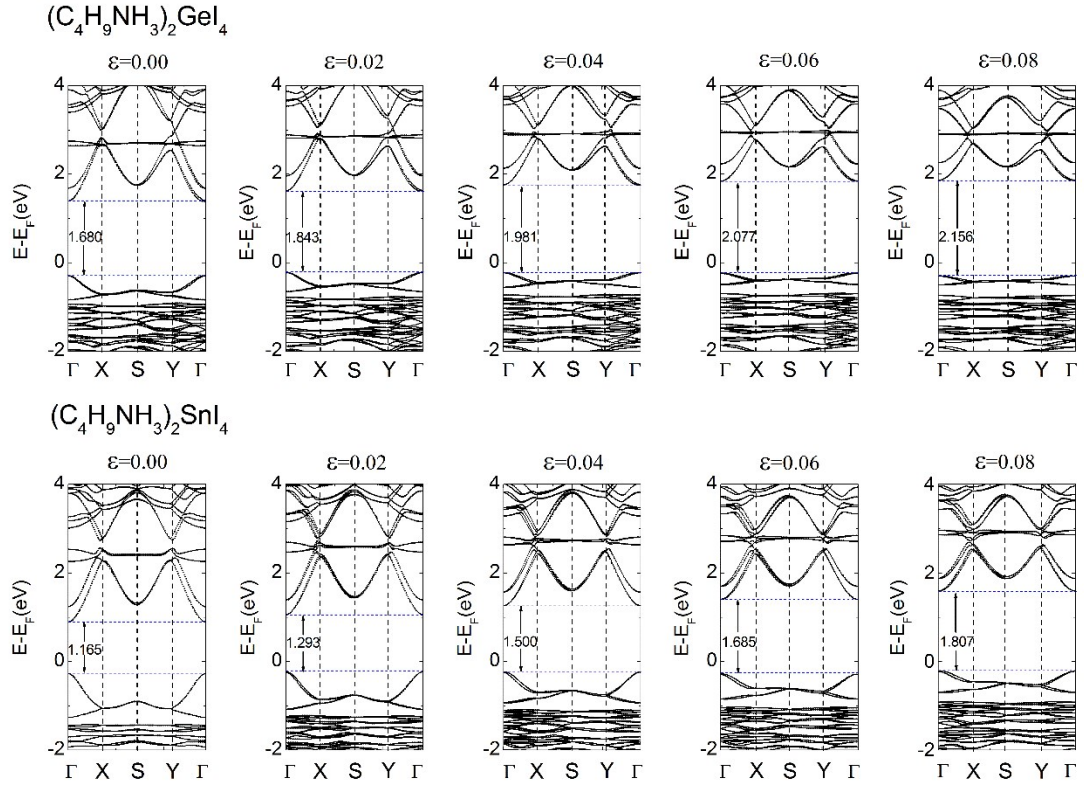


Fig. S3. Electronic band structures for monolayer $(\text{C}_4\text{H}_9\text{NH}_3)_2\text{GeI}_4$ and $(\text{C}_4\text{H}_9\text{NH}_3)_2\text{SnI}_4$, which is calculated by PBE-SOC.

(C4H9NH3)2GeI4 with space group C222 (No. 21), optimized with Grimme's D3 correction

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(C4H9NH3)2GeI4 with PBCA(No. 61) , optimized with Grimme's D3 correction

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0.9940821073878975 0.8435675025559944 0.6065732454387810
0.4940821073878972 0.8435675025559944 0.8934267545612190
0.5059178926121025 0.1564325384440057 0.1065732794387831
0.1054192587860313 0.5243398562629622 0.1817118074388694
0.8945807142139720 0.4756601437370441 0.8182881755611328
0.3945807412139682 0.4756601437370441 0.6817118244388672
0.6054192857860280 0.5243398562629622 0.3182881755611316
0.8945807142139720 0.0243398562629557 0.3182881755611316
0.1054192587860313 0.9756601437370378 0.6817118244388672
0.6054192857860280 0.9756601437370378 0.8182881755611328
0.3945807412139682 0.0243398562629557 0.1817118074388694
0.9520843793497707 0.3797542210243249 0.1792811243498919
0.0479156006502202 0.6202458059756742 0.8207188406501157

0.5479155646502317 0.6202458059756742 0.6792811593498843
0.4520843793497785 0.3797542210243250 0.3207188756501155
0.0479156006502202 0.8797541940243258 0.3207188756501155
0.9520843793497707 0.1202457789756741 0.6792811593498843
0.4520843793497785 0.1202457789756741 0.8207188406501157
0.5479155646502317 0.8797541940243258 0.1792811243498919
0.7499771632008072 0.6008548146788524 0.1869100054541303
0.2500228647991938 0.3991451583211621 0.8130899945458694
0.7500228367991928 0.3991451583211621 0.6869100054541306
0.2499771352008063 0.6008548146788524 0.3130899945458706
0.2500228647991938 0.1008548956788419 0.3130899945458706
0.7499771632008072 0.8991451313211432 0.6869100054541306
0.2499771352008063 0.8991451313211432 0.8130899945458694
0.7500228367991928 0.1008548956788419 0.1869100054541303
0.9032920493765354 0.7441822218940365 0.1896907020769273
0.0967079506234643 0.2558177511059720 0.8103092629230674
0.5967079506234646 0.2558177511059720 0.6896907370769326
0.4032920493765342 0.7441822218940365 0.3103092979230730
0.0967079506234643 0.2441822488940280 0.3103092979230730
0.9032920493765354 0.7558177781059635 0.6896907370769326
0.4032920493765342 0.7558177781059635 0.8103092629230674
0.5967079506234646 0.2441822488940280 0.1896907020769273
0.0076233582227012 0.6124756260387690 0.2659544164396592
0.9923766617773024 0.3875243739612314 0.7340455835603412
0.4923766417772992 0.3875243739612314 0.7659544164396588
0.5076233032226982 0.6124756260387690 0.2340455835603412
0.9923766617773024 0.1124755590387743 0.2340455835603412
0.0076233582227012 0.8875243739612310 0.7659544164396588
0.5076233032226982 0.8875243739612310 0.7340455835603412
0.4923766417772992 0.1124755590387743 0.2659544164396592
0.8514245095264151 0.4710215641017091 0.2634388615881763
0.1485754904735851 0.5289784898982802 0.7365611384118247
0.6485754904735849 0.5289784898982801 0.7634388615881753
0.3514245095264159 0.4710215641017091 0.2365611554118217
0.1485754904735851 0.9710215641017171 0.2365611554118217
0.8514245095264151 0.0289784358982909 0.7634388615881753
0.3514245095264159 0.0289784358982909 0.7365611384118247
0.6485754904735849 0.9710215641017171 0.2634388615881763
0.8093372766613548 0.6774853520632259 0.2730142339182245

0.1906627363386502	0.3225146479367739	0.7269857310817777
0.6906627233386452	0.3225146479367739	0.7730142689182223
0.3093372766613476	0.6774853520632259	0.2269857660817766
0.1906627363386502	0.1774852980632285	0.2269857660817766
0.8093372766613548	0.8225146479367741	0.7730142689182223
0.3093372766613476	0.8225146479367741	0.7269857310817777
0.6906627233386452	0.1774852980632285	0.2730142339182245
0.5679806183072752	0.0563559170503114	0.9470565113893222
0.4320194096927258	0.9436440559496820	0.0529435056106753
0.9320194376927223	0.9436440559496820	0.4470565463893285
0.0679805903072735	0.0563559170503114	0.5529434886106778
0.4320194096927258	0.5563559170503123	0.5529434886106778
0.5679806183072752	0.4436440829496884	0.4470565463893285
0.0679805903072735	0.4436440829496884	0.0529435056106753
0.9320194376927223	0.5563559170503122	0.9470565113893222
0.0000000000000000	0.0000000000000000	-0.0000000000000000
0.5000000000000000	0.0000000000000000	0.5000000000000000
0.0000000000000000	0.5000000000000000	0.5000000000000000
0.5000000000000000	0.5000000000000000	-0.0000000000000000

(C4H9NH3)2SnI4 with space group C222 (No. 21) , optimized with Grimme's D3 correction

1.0000000000000000		
8.3481558180763624	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.8101226461083808	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.9672069003488311
C	Sn	H I N
32	4	96 16 8

Direct

0.4888240893922437	0.0101898364331821	0.5075278813443166
0.4688244422764072	0.9294176434381468	0.4612156448388304
0.5265590483118503	0.0263724063952050	0.4206584622337960
0.4889512483949353	0.9524202133970908	0.3744026521544445
0.0111759016077586	0.4898101725668146	0.5075278813443166
0.0311755377235912	0.5705823565618532	0.4612156448388304
0.9734409816881451	0.4736275836047939	0.4206584622337960
0.0110487676050659	0.5475797866029092	0.3744026521544445
0.4888240893922437	0.5101898274331844	0.0075279023443150
0.4688244422764072	0.4294176154381457	0.9612156108388277

0.5265590483118503 0.5263724163952056 0.9206584282337937
0.4889512483949353 0.4524202133970885 0.8744026861544479
0.0111759016077586 0.9898101725668156 0.0075279023443150
0.0311755377235912 0.0705823635618565 0.9612156108388277
0.9734409816881451 0.9736275836047944 0.9206584282337937
0.0110487676050659 0.0475797906029115 0.8744026861544479
0.4888240893922437 0.9898101725668156 0.9924720856556842
0.4688244422764072 0.0705823635618565 0.0387843551611694
0.5265590483118503 0.9736275836047944 0.0793415547662020
0.4889512483949353 0.0475797906029115 0.1255973398455546
0.0111759016077586 0.5101898274331844 0.9924720856556842
0.0311755377235912 0.4294176154381457 0.0387843551611694
0.9734409816881451 0.5263724163952056 0.0793415547662020
0.0110487676050659 0.4524202133970885 0.1255973398455546
0.4888240893922437 0.4898101725668146 0.4924721186556832
0.4688244422764072 0.5705823565618532 0.5387843551611695
0.5265590483118503 0.4736275836047939 0.5793416047662054
0.4889512483949353 0.5475797866029092 0.6255973478455549
0.0111759016077586 0.0101898364331821 0.4924721186556832
0.0311755377235912 0.9294176434381468 0.5387843551611695
0.9734409816881451 0.0263724063952050 0.5793416047662054
0.0110487676050659 0.9524202133970908 0.6255973478455549
0.0068537217837049 0.0000000000000000 0.2500000000000000
0.4931462712162905 0.5000000000000000 0.2500000000000000
0.0068537217837049 0.5000000000000000 0.7499999830000021
0.4931462712162905 0.0000000000000000 0.7499999830000021
0.4169414277670155 0.1147394883140141 0.5088707181898924
0.6142915217651196 0.0426696894234452 0.5136582260353436
0.4513723199545785 0.9387257992475114 0.5366244302811429
0.3418132333941612 0.8993923185293023 0.4560686418561316
0.5353044361472636 0.8213072743195836 0.4614278107729038
0.6567604962927606 0.0457353380492938 0.4235283561692570
0.4694496244940474 0.1391268642176714 0.4219724999469290
0.3591868546301636 0.9442404700739486 0.3684619349061127
0.5402212557130809 0.8378449738567184 0.3713966462811488
0.5194934807076534 0.1575495997243657 0.3370398492431484
0.5258749988424171 -0.0009015373595904 0.3039550559647351
0.6821259902648354 0.0463829451328472 0.3372466649073712
0.0830585652329871 0.3852605046859885 0.5088707181898924

0.8857085082348829 0.4573303175765592 0.5136582260353436
0.0486276730454241 0.5612742007524886 0.5366244302811429
0.1581867816058440 0.6006076814706977 0.4560686418561316
0.9646955938527388 0.6786927256804164 0.4614278107729038
0.8432395337072419 0.4542646689507106 0.4235283561692570
0.0305503605059548 0.3608731217823281 0.4219724999469290
0.1408131453698362 0.5557595299260514 0.3684619349061127
0.9597787742869216 0.6621550261432816 0.3713966462811488
0.9805065292923474 0.3424503862756329 0.3370398492431484
0.9741250011575829 0.5009015373595903 0.3039550559647351
0.8178739797351621 0.4536170478671489 0.3372466649073712
0.4169414277670155 0.6147394953140095 0.0088706921898904
0.6142915217651196 0.5426696534234418 0.0136582230353483
0.4513723199545785 0.4387257432475123 0.0366244342811429
0.3418132333941612 0.3993922625293052 0.9560686078561278
0.5353044361472636 0.3213072743195755 0.9614278107729041
0.6567604962927606 0.5457353870492941 0.9235284231692595
0.4694496244940474 0.6391268502176699 0.9219724999469217
0.3591868546301636 0.4442404420739543 0.8684619019061126
0.5402212557130809 0.3378449738567175 0.8713966462811494
0.5194934807076534 0.6575496137243660 0.8370397822431465
0.5258749988424171 0.4990984626404094 0.8039550559647367
0.6821259902648354 0.5463829231328520 0.8372466309073611
0.0830585652329871 0.8852605046859905 0.0088706921898904
0.8857085082348829 0.9573303465765582 0.0136582230353483
0.0486276730454241 0.0612742357524890 0.0366244342811429
0.1581867816058440 0.1006077094706997 0.9560686078561278
0.9646955938527388 0.1786927116804234 0.9614278107729041
0.8432395337072419 0.9542646129507059 0.9235284231692595
0.0305503605059548 0.8608731497823301 0.9219724999469217
0.1408131453698362 0.0557595439260449 0.8684619019061126
0.9597787742869216 0.1621550401432836 0.8713966462811494
0.9805065292923474 0.8424503862756340 0.8370397822431465
0.9741250011575829 0.0009015473595909 0.8039550559647367
0.8178739797351621 0.9536170198671398 0.8372466309073611
0.4169414277670155 0.8852605046859905 0.9911292818101076
0.6142915217651196 0.9573303465765582 0.9863417739646564
0.4513723199545785 0.0612742357524890 0.9633755697188571
0.3418132333941612 0.1006077094706997 0.0439313581438687

0.5353044361472636 0.1786927116804234 0.0385721802270986
0.6567604962927606 0.9542646129507059 0.0764716358307422
0.4694496244940474 0.8608731497823301 0.0780275000530712
0.3591868546301636 0.0557595439260449 0.1315380730938887
0.5402212557130809 0.1621550401432836 0.1286033367188528
0.5194934807076534 0.8424503862756340 0.1629601677568567
0.5258749988424171 0.0009015473595909 0.1960449270352597
0.6821259902648354 0.9536170198671398 0.1627533690926316
0.0830585652329871 0.6147394953140095 0.9911292818101076
0.8857085082348829 0.5426696534234418 0.9863417739646564
0.0486276730454241 0.4387257432475123 0.9633755697188571
0.1581867816058440 0.3993922625293052 0.0439313581438687
0.9646955938527388 0.3213072743195755 0.0385721802270986
0.8432395337072419 0.5457353870492941 0.0764716358307422
0.0305503605059548 0.6391268502176699 0.0780275000530712
0.1408131453698362 0.4442404420739543 0.1315380730938887
0.9597787742869216 0.3378449738567175 0.1286033367188528
0.9805065292923474 0.6575496137243660 0.1629601677568567
0.9741250011575829 0.4990984626404094 0.1960449270352597
0.8178739797351621 0.5463829231328520 0.1627533690926316
0.4169414277670155 0.3852605046859885 0.4911292818101073
0.6142915217651196 0.4573303175765592 0.4863417739646543
0.4513723199545785 0.5612742007524886 0.4633755697188651
0.3418132333941612 0.6006076814706977 0.5439313581438694
0.5353044361472636 0.6786927256804164 0.5385721892270959
0.6567604962927606 0.4542646689507106 0.5764716108307433
0.4694496244940474 0.3608731217823281 0.5780274670530792
0.3591868546301636 0.5557595299260514 0.6315380650938882
0.5402212557130809 0.6621550261432816 0.6286033197188549
0.5194934807076534 0.3424503862756329 0.6629601837568507
0.5258749988424171 0.5009015373595903 0.6960449100352605
0.6821259902648354 0.4536170478671489 0.6627533350926361
0.0830585652329871 0.1147394883140141 0.4911292818101073
0.8857085082348829 0.0426696894234452 0.4863417739646543
0.0486276730454241 0.9387257992475114 0.4633755697188651
0.1581867816058440 0.8993923185293023 0.5439313581438694
0.9646955938527388 0.8213072743195836 0.5385721892270959
0.8432395337072419 0.0457353380492938 0.5764716108307433
0.0305503605059548 0.1391268642176714 0.5780274670530792

0.1408131453698362	0.9442404700739486	0.6315380650938882
0.9597787742869216	0.8378449738567184	0.6286033197188549
0.9805065292923474	0.1575495997243657	0.6629601837568507
0.9741250011575829	-0.0009015373595904	0.6960449100352605
0.8178739797351621	0.0463829451328472	0.6627533350926361
0.9906242729891068	0.9417422514356215	0.1417573650173047
0.5093757570108957	0.5582577485643785	0.1417573650173047
0.2500000000000000	0.2500000000000000	0.2297887473476201
0.2500000000000000	0.7500000000000000	0.2702112526523798
0.7500000149999977	0.2500000000000000	0.2352657549089320
0.7500000149999977	0.7500000000000000	0.2647342610910692
0.9906242729891068	0.0582577515643820	0.3582426179826909
0.5093757570108957	0.4417422514356216	0.3582426179826909
0.9906242729891068	0.4417422514356216	0.6417573480173063
0.5093757570108957	0.0582577515643821	0.6417573480173063
0.2500000000000000	0.7500000000000000	0.7297887803476184
0.2500000000000000	0.2500000000000000	0.7702112526523808
0.7500000149999977	0.7500000000000000	0.7352658059089323
0.7500000149999977	0.2500000000000000	0.7647342280910705
0.9906242729891068	0.5582577485643785	0.8582426179826909
0.5093757570108957	0.9417422514356215	0.8582426179826909
0.5570955339383484	0.0443694517215608	0.3354927588817444
0.9429044360616491	0.4556305412784351	0.3354927588817444
0.5570955339383484	0.5443694867215672	0.8354927258817448
0.9429044360616491	0.9556305692784375	0.8354927258817448
0.5570955339383484	0.9556305692784375	0.1645072411182557
0.9429044360616491	0.5443694867215672	0.1645072411182557
0.5570955339383484	0.4556305412784350	0.6645073081182580
0.9429044360616491	0.0443694517215608	0.6645073081182580

(C4H9NH3)2SnI4 with PBCA(No. 61) , optimized with Grimme's D3 correction

1.0000000000000000		
8.6663874285669795	-0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5284427959949820	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.0125808126772355
I	N	C
16	8	32
96	4	

Direct

0.0227271064984260	0.0093957054401794	0.1142378515649196
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0.9772729525015689 0.9906042625598149 0.8857621404350804
0.4772728695015722 0.9906042625598149 0.6142378595649196
0.5227271024984250 0.0093957054401794 0.3857621404350793
0.9772729525015689 0.5093956834401877 0.3857621404350793
0.0227271064984260 0.4906043165598166 0.6142378595649196
0.5227271024984250 0.4906043165598166 0.8857621404350804
0.4772728695015722 0.5093956834401877 0.1142378515649196
0.1927475185642026 0.6911017703522577 0.9976639176943518
0.8072524674358050 0.3088982566477447 0.0023360893056455
0.3072524954357979 0.3088982566477447 0.4976639176943505
0.6927475325641950 0.6911017703522577 0.5023361163056439
0.8072524674358050 0.1911017573522552 0.5023361163056439
0.1927475185642026 0.8088982296477423 0.4976639176943505
0.6927475325641950 0.8088982296477423 0.0023360893056455
0.3072524954357979 0.1911017573522552 0.9976639176943518
0.0805108862757225 0.4190915609187042 0.0929990218365008
0.9194890647242784 0.5809084930812924 0.9070009691634945
0.4194891197242772 0.5809084930812924 0.5929990308365055
0.5805109352757216 0.4190915609187042 0.4070009691634937
0.9194890647242784 0.9190915609187049 0.4070009691634937
0.0805108862757225 0.0809084460812921 0.5929990308365055
0.5805109352757216 0.0809084460812921 0.9070009691634945
0.4194891197242772 0.9190915609187049 0.0929990218365008
0.9676233412216192 0.5237514496365123 0.1178636290886263
0.0323766277783739 0.4762485503634809 0.8821363449113722
0.5323766587783808 0.4762485503634809 0.6178636550886278
0.4676233682216251 0.5237514496365123 0.3821363799113714
0.0323766277783739 0.0237514646365247 0.3821363799113714
0.9676233412216192 0.9762485503634877 0.6178636550886278
0.4676233682216251 0.9762485503634877 0.8821363449113722
0.5323766587783808 0.0237514646365247 0.1178636290886263
0.9811045579624498 0.5082795632805811 0.1718089114022292
0.0188954200375487 0.4917204367194180 0.8281910885977710
0.5188954420375502 0.4917204367194180 0.6718089114022290
0.4811045579624491 0.5082795632805811 0.3281910885977717
0.0188954200375487 0.0082795812805767 0.3281910885977717
0.9811045579624498 0.9917204367194189 0.6718089114022290
0.4811045579624491 0.9917204367194189 0.8281910885977710
0.5188954420375502 0.0082795812805767 0.1718089114022292

0.8704614704408730 0.6196449220005731 0.1975982046573599
0.1295385155591266 0.3803550509994202 0.8024017603426442
0.6295385295591270 0.3803550509994202 0.6975982396573558
0.3704614704408725 0.6196449220005731 0.3024017953426410
0.1295385155591266 0.1196448880005782 0.3024017953426410
0.8704614704408730 0.8803550779994269 0.6975982396573558
0.3704614704408725 0.8803550779994269 0.8024017603426442
0.6295385295591270 0.1196448880005782 0.1975982046573599
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