

Supporting Information

N-, B-, P-, Al-, As-, Ga-graphdiyne/graphyne lattices; First-principles investigation of mechanical, optical and electronic properties

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1. Atomic structures of constructed monolayers unit-cells in VASP POSCAR.
- 2-AIMD results for the thermal stability
- 3- HSE06 results for the total electronic density of states.

N-GD-Hex.

1.000000000000000		
16.0375168077986103	0.000000000000000	0.000000000000000
8.0187584038993034	13.8888969726305600	0.000000000000000
0.000000000000000	0.000000000000000	20.000000000000000

C	N
18	6

Direct

0.3804121860736274	0.3804121974542980	0.500000000000000
0.4316795762031731	0.4316795914129870	0.500000000000000
0.4757496464837061	0.4757496360660340	0.500000000000000
0.5242503541734678	0.5242503770415965	0.500000000000000
0.5683204244540008	0.5683204216946365	0.500000000000000
0.6195877851269032	0.6195878156533254	0.500000000000000
0.2391756153880706	0.3804121974542980	0.500000000000000
0.3804121899027848	0.2391756250017565	0.500000000000000
0.6195878141557571	0.7608243813031450	0.500000000000000
0.7608243499211298	0.6195878156533254	0.500000000000000
0.5683204201970540	0.8633591692205371	0.500000000000000
0.5242503755440140	0.9514992585266029	0.500000000000000
0.4316795872628418	0.1366408302816495	0.500000000000000
0.4757496319158818	0.0485007409755767	0.500000000000000
0.1366429261230877	0.4316795846102650	0.500000000000000
0.0485049320680702	0.4757496292633121	0.500000000000000
0.8633570459888276	0.5683204148919145	0.500000000000000
0.9514950400438522	0.5242503702388746	0.500000000000000
0.2833474513407666	0.4333051021258214	0.500000000000000
0.4333050907451508	0.2833474588922726	0.500000000000000
0.2833474492785868	0.2833474588922726	0.500000000000000
0.5666948838567194	0.7166525474126288	0.500000000000000
0.7166525493164073	0.5666949109818020	0.500000000000000
0.7166525194319675	0.7166525474126288	0.500000000000000

N-GY-Hex.

11.5797873518352397	0.0000000000000000	0.0000000000000000
5.7898936759176269	10.0283900171084106	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C N

12 6

Direct

0.3975461511808547	0.3987924258657713	0.5000000000000000
0.4685431739356289	0.4702748313915350	0.5000000000000000
0.6006470415036986	0.6018240656336928	0.5000000000000000
0.5291969403822065	0.5308089384523669	0.5000000000000000
0.2024805047568350	0.3981648927816792	0.5000000000000000
0.3981417432226024	0.2030826264798407	0.5000000000000000
0.6012319802712014	0.7969027701085238	0.5000000000000000
0.7963442103420633	0.6011940784531404	0.5000000000000000
0.5302420982084755	0.9394030545548517	0.5000000000000000
0.4696462107871966	0.0605897311760231	0.5000000000000000
0.0600113572813541	0.4691801693066679	0.5000000000000000
0.9388256734944491	0.5296969456450924	0.5000000000000000
0.2632619341083853	0.4716467956766834	0.5000000000000000
0.4709938337485937	0.2645160471613082	0.5000000000000000
0.2638737991634841	0.2638794235391089	0.5000000000000000
0.5277589604892654	0.7361099311326029	0.5000000000000000
0.7349096043595935	0.5283397175771967	0.5000000000000000
0.7355193567640583	0.7354666850638765	0.5000000000000000

N-GD-Rec.

1.0000000000000000

9.6700000762999991	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.970000266999996	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C N

24 4

Direct

0.10300000000000015	0.0890000019999988	0.5000000000000000
0.17800000300000011	0.1640000049999983	0.5000000000000000
0.2430000009999986	0.2300000039999972	0.5000000000000000
0.31400001000000009	0.30300000300000011	0.5000000000000000
0.3790000079999984	0.3689999879999988	0.5000000000000000
0.45399999600000003	0.44400000600000031	0.5000000000000000
0.95399999600000003	0.0890000019999988	0.5000000000000000
0.8790000079999984	0.1640000049999983	0.5000000000000000
0.81400001000000009	0.2300000039999972	0.5000000000000000
0.74299997100000033	0.30300000300000011	0.5000000000000000
0.6779999729999986	0.3689999879999988	0.5000000000000000
0.6029999849999967	0.44400000600000031	0.5000000000000000
0.45399999600000003	0.58899998700000011	0.5000000000000000
0.3790000079999984	0.66399997500000030	0.5000000000000000
0.31400001000000009	0.73000001900000020	0.5000000000000000
0.2430000009999986	0.8029999729999986	0.5000000000000000
0.17800000300000011	0.86900001800000013	0.5000000000000000
0.10300000000000015	0.94400000600000031	0.5000000000000000
0.6029999849999967	0.58899998700000011	0.5000000000000000
0.6779999729999986	0.66399997500000030	0.5000000000000000
0.74299997100000033	0.73000001900000020	0.5000000000000000
0.81400001000000009	0.8029999729999986	0.5000000000000000
0.8790000079999984	0.86900001800000013	0.5000000000000000
0.95399999600000003	0.94400000600000031	0.5000000000000000
0.17499999700000005	0.01600000100000019	0.5000000000000000
0.8820000289999967	0.01600000100000019	0.5000000000000000
0.38199999900000014	0.5159999729999996	0.5000000000000000
0.6750000119999982	0.5159999729999996	0.5000000000000000

N-GY-Rec.

1.000000000000000		
7.0518848930517954	0.000000000000000	0.000000000000000
0.000000000000000	11.5450439196077035	0.000000000000000
0.000000000000000	0.000000000000000	20.000000000000000

C N

16 4

Direct

0.1391125793967873	0.1235654885620434	0.500000000000000
0.9347703032909891	0.1235659594382170	0.500000000000000
0.2429134365813752	0.2281861732100054	0.500000000000000
0.8309662910531941	0.2281855003073119	0.500000000000000
0.3309721022024235	0.3193156587373949	0.500000000000000
0.7429047944840406	0.3193139794365294	0.500000000000000
0.4347694865073137	0.4239371360481385	0.500000000000000
0.6391110308108736	0.4239370473975370	0.500000000000000
0.4347703249608159	0.6235647245859965	0.500000000000000
0.6391117186747195	0.6235650809339219	0.500000000000000
0.3309732943633961	0.7281871673125337	0.500000000000000
0.7429060847906044	0.7281879216405684	0.500000000000000
0.2429121988745067	0.8193157822493404	0.500000000000000
0.8309644509210514	0.8193175505700410	0.500000000000000
0.1391113567533750	0.9239359318246798	0.500000000000000
0.9347687722682707	0.9239367911429142	0.500000000000000
0.8367555659106998	0.0237512760830541	0.500000000000000
0.2371281563175671	0.0237508141460694	0.500000000000000
0.3367532281006902	0.5237515600530287	0.500000000000000
0.7371302038786638	0.5237504028537643	0.500000000000000

B-GD-Hex

1.0000000000000000		
11.8467556014048103	0.0000000000000000	0.0000000000000000
5.9233778007024069	10.2595913032290600	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C B

12 2

Direct

0.4070308672173653	0.1859346011964433	0.5000000006440217
0.4672015211373619	0.0655895691018387	0.5000000029657059
0.4070311110582381	0.4070304009524435	0.4999999994757971
0.4672009784262485	0.4672011005079426	0.5000000001081091
0.5327928226503715	0.5327934736097859	0.5000000019487061
0.5929670091187731	0.5929683745784118	0.5000000023988420
0.5929644137274650	0.8140626494910990	0.4999999968751183
0.5327933412711943	0.9344053481882924	0.4999999985596588
0.1859349549626330	0.4070305223908619	0.5000000039912749
0.0655896108587868	0.4672031250811983	0.4999999994225561
0.8140623904039757	0.5929635621580545	0.4999999967410673
0.9344050922340088	0.5327923036735314	0.4999999982217460
0.3333309009287149	0.3333311806515624	0.5000000025095019
0.6666637191866585	0.6666639905117151	0.4999999961379018

B-GY-Hex.

1.0000000000000000		
7.3993340266393819	0.0000000000000000	0.0000000000000000
3.6996670133196909	6.4080112381514613	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C B

6 2

Direct

0.5479762480075649	0.9039220011690006	0.5000000793771591
0.5479869980626120	0.5479852524329090	0.4999999399615902
0.4519468433367706	0.4519467250748832	0.4999999686695276
0.4520326477347396	0.0960011329332673	0.4999998768714633
0.9039167495750249	0.5479814554799134	0.5000000725807894
0.0960060592445231	0.4520289232261874	0.5000001081962822
0.3333059913196195	0.3333054936785800	0.5000001525667130
0.6666298759498659	0.6666305724160608	0.4999998017764611

```

singlepoint
  B-GD-Rec.
    15.1176650848092127    0.0000000000000000    0.0000000000000000
    0.0000000000000000    11.5612740620846104    0.0000000000000000
    0.0000000000000000    0.0000000000000000    20.0000000000000000
  C      B
    22      2
Direct
0.4102543203183444  0.4972997911539707  0.4999943875085933
0.4919637545246118  0.4970378879462274  0.4999940130849367
0.0835927457478149  0.9973498433664432  0.5000095736013748
0.5808820385932378  0.4972124811580088  0.4999599154717203
0.6625666286417982  0.4979044381627347  0.4999522700811241
0.8129567423530801  0.6107869238143309  0.5000175685562596
0.8541040797492556  0.7031882062001102  0.5000189915735689
0.8994224109006836  0.8029757052982518  0.5000033702213997
0.9417467152681525  0.8940659224030654  0.4999986036754152
0.8124522838408836  0.3849345856775699  0.5000014716709060
0.8537998614889659  0.2926848723814501  0.5000045507176125
0.8995672581886254  0.1932835705093723  0.5000075365614407
0.9422300136765998  0.1024618047785353  0.5000108351598911
0.9893746828101939  0.9979912298404514  0.5000120512789721
0.2600157029430008  0.6101205945504731  0.4999991645283117
0.2189736087037986  0.7025882507091126  0.5000012457462049
0.1736745103528392  0.8023807938007934  0.5000142302960171
0.1308458105754013  0.8930956778439594  0.5000139850056300
0.2603278219382759  0.3842164513274966  0.5000008628663153
0.2190016690507264  0.2919763568140610  0.4999997481206933
0.1737068959249086  0.1922734938699264  0.4999995814372298
0.1311633460361961  0.1013913330666938  0.5000006670304842
0.3102668156786805  0.4972810803439316  0.4999980839611595
0.7625361889960516  0.4980490806622413  0.4999897363013588

```

B-GY-Rec.

1.000000000000000

9.9118335633718662 0.000000000000000 0.000000000000000

0.000000000000000 7.1456395344936281 0.000000000000000

0.000000000000000 0.000000000000000 20.000000000000000

C B

12 2

Direct

0.4436304256107917 0.4977387292673399 0.5000007394621164

0.5678475347842138 0.4979349552453982 0.5000018864417797

0.7973140674481201 0.6820363819270483 0.5000027950606594

0.0769959974217684 0.9972719175965992 0.5000018115432567

0.8612945539651733 0.8292139281396160 0.5000029907859656

0.7981220739329871 0.3155363053877949 0.4999904995003064

0.8621625230843861 0.1683925052963104 0.4999942627648863

0.9343430405121111 0.9984003996479487 0.5000002624103104

0.1491270017164865 0.8273009720484268 0.5000015666116582

0.2134506872780619 0.6803162790984132 0.5000017468919111

0.2141025678304445 0.3136742697527382 0.5000013707553776

0.1501440171308133 0.1664009924425898 0.5000008796302637

0.2905275792049409 0.4972472270730606 0.5000011074140289

0.7209377640796788 0.4985351370766722 0.4999981997274858

P-GD-Hex.

1.0000000000000000		
17.0762411269667496	0.0000000000000000	0.0000000000000000
8.5381205634936137	14.7884586170697698	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	P
18	6

Direct

0.3883440430082246	0.3883440543888952	0.5000000000000000
0.4356299059855715	0.4356299211953782	0.5000000000000000
0.4773877227866876	0.4773877123690156	0.5000000000000000
0.5226122778704934	0.5226123007386150	0.5000000000000000
0.5643700946716095	0.5643700919122452	0.5000000000000000
0.6116559281923060	0.6116559587187282	0.5000000000000000
0.2233119015188478	0.3883440543888952	0.5000000000000000
0.3883440468373820	0.2233119111325337	0.5000000000000000
0.6116559572211600	0.7766880951723678	0.5000000000000000
0.7766880637903526	0.6116559587187282	0.5000000000000000
0.5643700904146627	0.8712598287853623	0.5000000000000000
0.5226122992410325	0.9547754111325588	0.5000000000000000
0.4356299170452402	0.1287401707168243	0.5000000000000000
0.4773877082188562	0.0452245883696207	0.5000000000000000
0.1287422665582625	0.4356299143926563	0.5000000000000000
0.0452287794621142	0.4773877055662865	0.5000000000000000
0.8712577055536528	0.5643700851095232	0.5000000000000000
0.9547711926498081	0.5226122939358930	0.5000000000000000
0.2698763468212846	0.4602473111648067	0.5000000000000000
0.4602472997841289	0.2698763543727907	0.5000000000000000
0.2698763447591048	0.2698763543727907	0.5000000000000000
0.5397526748177341	0.7301236519321108	0.5000000000000000
0.7301236538358893	0.5397527019428168	0.5000000000000000
0.7301236239514495	0.7301236519321108	0.5000000000000000

P-GD-Rec.

1.000000000000000

9.9016546045490905 0.000000000000000 0.000000000000000

0.000000000000000 16.7570655905802965 0.000000000000000

0.000000000000000 0.000000000000000 20.000000000000000

C P

24 4

Direct

0.1011057073697543 0.0996759729666508 0.500000000000000

0.1715359387340740 0.1720553342319917 0.500000000000000

0.2409639890193844 0.2332865160045898 0.500000000000000

0.3156331645583990 0.2998551476247684 0.500000000000000

0.3854864552872002 0.3609163416227830 0.500000000000000

0.4561735613616449 0.4333006158390376 0.500000000000000

0.9560344620600958 0.0996304136617994 0.500000000000000

0.8853592698181743 0.1719518630405403 0.500000000000000

0.8159310959978043 0.2331745802463701 0.500000000000000

0.7413755650225227 0.2997852240750589 0.500000000000000

0.6717749756217017 0.3609307823496479 0.500000000000000

0.6012841819335435 0.4333557057693014 0.500000000000000

0.4560297745255966 0.5996310039083568 0.500000000000000

0.3853614553452758 0.6719521972960862 0.500000000000000

0.3159333890186602 0.7331738203378606 0.500000000000000

0.2413802865005295 0.7997838472512271 0.500000000000000

0.1717687887552444 0.8609282538431913 0.500000000000000

0.1012863573383029 0.9333533101445610 0.500000000000000

0.6011055244022714 0.5996784488043119 0.500000000000000

0.6715345020313563 0.6720563200839038 0.500000000000000

0.7409622434022225 0.7332885256840100 0.500000000000000

0.8156317951030445 0.7998550946903009 0.500000000000000

0.8854878320137871 0.8609164612213718 0.500000000000000

0.9561809551118401 0.9332972028209383 0.500000000000000

0.2102592774527565 0.0165785241968237 0.500000000000000

0.8470914901515840 0.0164415185264630 0.500000000000000

0.3470655692375999 0.5164483757043357 0.500000000000000

0.7102616211036477 0.5165784477335364 0.500000000000000

P-GY-Hex.

1.000000000000000		
12.6229910288837601	0.000000000000000	0.000000000000000
6.3114955144317930	10.9318309027610496	0.000000000000000
0.000000000000000	0.000000000000000	20.000000000000000

C P

12 6

Direct

0.4068769953922455	0.4077887264159088	0.500000000000000
0.4708488244327640	0.4722500769184208	0.500000000000000
0.5916282293481316	0.5924481093858631	0.500000000000000
0.5272720803400617	0.5283916065036465	0.500000000000000
0.1840848011310001	0.4075379814033155	0.500000000000000
0.4072386715099725	0.1847145888653614	0.500000000000000
0.5919628563713886	0.8152678490382428	0.500000000000000
0.8146739385600341	0.5921950533056162	0.500000000000000
0.5277258498210742	0.9437157009366359	0.500000000000000
0.4714491650206156	0.0562691073688129	0.500000000000000
0.0556722166738908	0.4715935633984714	0.500000000000000
0.9431075259947548	0.5277367575201311	0.500000000000000
0.2468176537094138	0.5048275259978681	0.500000000000000
0.5042562568563085	0.2477620427181080	0.500000000000000
0.2472036282296060	0.2474710253979353	0.500000000000000
0.4946804470731792	0.7525176776653097	0.500000000000000
0.7516502826402771	0.4951606832524291	0.500000000000000
0.7520251508952356	0.7522250539079280	0.500000000000000

P-GY-Rec.

1.0000000000000000

7.3137354342499892 0.0000000000000000 0.0000000000000000

0.0000000000000000 12.3515344376282865 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C P

16 4

Direct

0.1348550644560760 0.1373659798560709 0.5000000000000000

0.9389822434174633 0.1373511698424394 0.5000000000000000

0.2353740545448346 0.2343020405173419 0.5000000000000000

0.8383968685807517 0.2342723630785173 0.5000000000000000

0.3382980502687047 0.3131770367896962 0.5000000000000000

0.7356658877880378 0.3132341615161423 0.5000000000000000

0.4389952145876563 0.4101071227546171 0.5000000000000000

0.6349542895259077 0.4101333959952100 0.5000000000000000

0.4389821888442711 0.6373505085721618 0.5000000000000000

0.6348534307204758 0.6373660491197484 0.5000000000000000

0.3383972432336009 0.7342725397089325 0.5000000000000000

0.7353622838369773 0.7343026641163561 0.5000000000000000

0.2356662625078698 0.8132337069685818 0.5000000000000000

0.8382972994721456 0.8131798178522942 0.5000000000000000

0.1349537495950059 0.9101332503120361 0.5000000000000000

0.9389945578386545 0.9101042200009388 0.5000000000000000

0.7931695959405332 0.0237729417586081 0.5000000000000000

0.2807187867022236 0.0237949666050952 0.5000000000000000

0.2931694837509013 0.5237728125613828 0.5000000000000000

Al-GD-Hex.

1.0000000000000000

13.1909355616628208 0.0000000000000000 0.0000000000000000

6.5954677808314059 11.4236852960858908 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C Al

12 2

Direct

0.4163193831818788 0.1673483647599809 0.5000000131005322

0.4703959001774578 0.0591940881052437 0.5000000011250449

0.4163244879008516 0.4163246158849532 0.5000000022842883

0.4704010583121416 0.4704021715942730 0.5000000045760018

0.5295962229974407 0.5295967185057009 0.5000000023231479

0.5836729962168263 0.5836739418026795 0.4999999903051418

0.5836701608369381 0.8326496696282462 0.4999999898918404

0.5295937824946861 0.9408040318116662 0.4999999957134378

0.1673480265751550 0.4163184540264737 0.5000000204493276

0.0591941839563148 0.4703954020424490 0.5000000017307471

0.8326504397857661 0.5836710904234508 0.4999999861182900

0.9408043777263373 0.5295943561425318 0.4999999916007667

0.3333316287571364 0.3333326276806901 0.5000000121946897

0.6666660842628787 0.6666646696848701 0.4999999885867723

Al-GD-Rec.

1.000000000000000

16.6913823920642486 0.000000000000000 0.000000000000000

0.000000000000000 11.9797222550346518 0.000000000000000

0.000000000000000 0.000000000000000 20.000000000000000

C Al

22 2

Direct

0.4219181421271045	0.4968755553836743	0.4999246596841544
0.4959299842145555	0.4962142310438438	0.4999955020006936
0.0788338997709985	0.9973470768461539	0.5000135657885565
0.5769815696023528	0.4961664718089551	0.5000041197425915
0.6510001852978036	0.4967302497601196	0.4999734396540205
0.8219968889840956	0.6342243228719084	0.4999866338689571
0.8634066001432217	0.7198497880848223	0.4999663343287963
0.9086977515031762	0.8127741203667114	0.4999658216716156
0.9503897135472528	0.8974296339823979	0.4999752093003380
0.8239663951807330	0.3629781382413810	0.5000024302580712
0.8648448934725721	0.2768155995628376	0.5000097993589705
0.9092637821454161	0.1829009148210901	0.5000140286133501
0.9503940087778560	0.0976707685996558	0.5000130042156883
0.9940959781275112	0.9975129286031574	0.5000009365843709
0.2505929076811029	0.6338339839315026	0.5000149691215157
0.2092242367844008	0.7194786766509083	0.5000033238073698
0.1640143579730733	0.8124625644244290	0.4999833507396829
0.1223084792095221	0.8970790364064314	0.4999668782468589
0.2493121958328928	0.3625504885007871	0.5000067475907883
0.2084686458768132	0.2763296962743240	0.5000358369025051
0.1640354138962508	0.1824009177090034	0.5000812133775199
0.1228063813985898	0.0972557341553113	0.5000818648311736
0.3083615873967176	0.4978026929102484	0.4999876398680740
0.7645819073581137	0.4978667847395499	0.4999951349009493

Al-GY-Hex.

1.000000000000000		
8.7385998001500145	0.0000000000000000	0.0000000000000000
4.3692999000750072	7.5678494204324851	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C Al
6 2

Direct

0.4592508384133325	0.0814847470073943	0.5000000398785929
0.4592029139166840	0.4591992593795240	0.4999999170624889
0.5407249369640752	0.5407281158476422	0.4999997718193043
0.5407788986599016	0.9184351162108015	0.4999997995409018
0.0814853102600708	0.4592521983274338	0.5000004003909169
0.9184353729581787	0.5407789530123850	0.5000001177757909
0.3332946044703391	0.3332935751057491	0.5000003021765949
0.6666285375881387	0.6666295915199285	0.4999996513553810

Al-GY-Rec.

1.000000000000000		
11.1529645605559509	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.7685626894044466	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C Al
12 2

Direct

0.4499939922738108	0.4990567800341452	0.4999823215509451
0.5606381289406031	0.4987630640948026	0.4999835213199546
0.8186997027491074	0.7080147209288015	0.5000191346320193
0.0687631523502148	0.9976849550740923	0.4999986828312615
0.8773093986876574	0.8421449312582894	0.5000193122154784
0.8177384804321264	0.2869955303253846	0.5000011805333813
0.8769994424861025	0.1534468435293235	0.5000013667184078
0.9428771044048005	0.9979027378997003	0.5000059180591450
0.1341289499526397	0.8417332550358907	0.4999997685222013
0.1933778721341852	0.7082260158376883	0.5000001174351638
0.1936714625405500	0.2869268423776177	0.4999966598797911
0.1345988294584330	0.1531965743132986	0.4999943256496593
0.2795925891399662	0.4979291953326239	0.499996286490976
0.7316107284497875	0.4979785539582693	0.5000015231616146

As-GD-Hex.

1.0000000000000000		
17.4431125901974795	0.0000000000000000	0.0000000000000000
8.7215562951091812	15.1061786241503899	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	As
18	6

Direct

0.3910489357898683	0.3910489471705461	0.5000000000000000
0.4368419442604932	0.4368419594703070	0.5000000000000000
0.4779532924598939	0.4779532820422290	0.5000000000000000
0.5220467081972728	0.5220467310653945	0.5000000000000000
0.5631580563966807	0.5631580536373164	0.5000000000000000
0.6089510354106551	0.6089510659370774	0.5000000000000000
0.2179021159556100	0.3910489471705461	0.5000000000000000
0.3910489396190329	0.2179021255692959	0.5000000000000000
0.6089510644395091	0.7820978807356056	0.5000000000000000
0.7820978493535904	0.6089510659370774	0.5000000000000000
0.5631580521397339	0.8736839053351844	0.5000000000000000
0.5220467295678120	0.9559065504789857	0.5000000000000000
0.4368419553201619	0.1263160941669952	0.5000000000000000
0.4779532778920697	0.0440934490231939	0.5000000000000000
0.1263181900084334	0.4368419526675851	0.5000000000000000
0.0440976401156874	0.4779532752395070	0.5000000000000000
0.8736817821034748	0.5631580468345945	0.5000000000000000
0.9559023319962350	0.5220467242626725	0.5000000000000000
0.2661038370196209	0.4677923307681482	0.5000000000000000
0.4677923193874776	0.2661038445711270	0.5000000000000000
0.2661038349574412	0.2661038445711270	0.5000000000000000
0.5322076552143926	0.7338961617337745	0.5000000000000000
0.7338961636375529	0.5322076823394752	0.5000000000000000
0.7338961337531131	0.7338961617337745	0.5000000000000000

As-GD-Rec.

1.000000000000000		
10.0916634603880642	0.000000000000000	0.000000000000000
0.000000000000000	17.0110213075002790	0.000000000000000
0.000000000000000	0.000000000000000	20.000000000000000

C	As
24	4

Direct

0.0991195475620543	0.1044644167345012	0.500000000000000
0.1702681748609862	0.1747051167527829	0.500000000000000
0.2413438929285832	0.2339704709958070	0.500000000000000
0.3166946359900251	0.2986313461103265	0.500000000000000
0.3869663897236819	0.3582314515281055	0.500000000000000
0.4576714421416312	0.4285863852871401	0.500000000000000
0.9576953201756737	0.1044747610529271	0.500000000000000
0.8868496936336285	0.1748173947668192	0.500000000000000
0.8163826849392564	0.2343339686139458	0.500000000000000
0.7409330581315103	0.2989312559314072	0.500000000000000
0.6700401978831678	0.3582629599565905	0.500000000000000
0.5991004559386965	0.4285859819191202	0.500000000000000
0.4576808617125607	0.6044734582954661	0.500000000000000
0.3868329202527505	0.6747961486132894	0.500000000000000
0.3163648521629980	0.7343241660292392	0.500000000000000
0.2409171227182156	0.7989242712928046	0.500000000000000
0.1700278300077187	0.8582773527767813	0.500000000000000
0.0991128471652161	0.9286020036029612	0.500000000000000
0.5991362994748997	0.6044673060339534	0.500000000000000
0.6702657812147166	0.6747114582339222	0.500000000000000
0.7413443035205987	0.7339705076730496	0.500000000000000
0.8166955454890683	0.7986233435897816	0.500000000000000
0.8869676483798514	0.8582277738569388	0.500000000000000
0.9577022820420424	0.9285917846802718	0.500000000000000
0.2163952620891223	0.0165103961462592	0.500000000000000
0.8405760800537507	0.0164467282225829	0.500000000000000
0.3405767734927494	0.5164475812064069	0.500000000000000
0.7163373245927147	0.5164900597765580	0.500000000000000

As-GY-Hex.

1.0000000000000000		
12.9938772976492896	0.0000000000000000	0.0000000000000000
6.4969386488142700	11.2530278334269500	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	As
12	6

Direct

0.4086025158527136	0.4123646835437427	0.5000000000000000
0.4696076181900679	0.4747210283805927	0.5000000000000000
0.5869749856656483	0.5908098138874749	0.5000000000000000
0.5245822655128549	0.5298673047348359	0.5000000000000000
0.1777931722900448	0.4091922957249352	0.5000000000000000
0.4117488727315148	0.1783028623873122	0.5000000000000000
0.5902276200343692	0.8216354777034596	0.5000000000000000
0.8209911381259971	0.5876339312557803	0.5000000000000000
0.5291613952247260	0.9449276588628734	0.5000000000000000
0.4740591000504040	0.0550108820137609	0.5000000000000000
0.0544653341174595	0.4701358810706324	0.5000000000000000
0.9443476435161102	0.5252485214640075	0.5000000000000000
0.2408688199638505	0.5134768145436652	0.5000000000000000
0.5128621418511727	0.2449950910584207	0.5000000000000000
0.2445430251162435	0.2413377896080888	0.5000000000000000
0.4859425716341335	0.7587010057223509	0.5000000000000000
0.7543449449956867	0.4865301120564212	0.5000000000000000
0.7580514091270132	0.7549819759816572	0.5000000000000000

As-GY-Rec.

1.0000000000000000		
7.4389940700838864	0.0000000000000000	0.0000000000000000
0.0000000000000000	12.6650232932029194	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C As

16 4

Direct

0.1324521476419847	0.1431930693205956	0.5000000000000000
0.9410332511764565	0.1431465625538308	0.5000000000000000
0.2341123612682168	0.2361151848375087	0.5000000000000000
0.8396876111876779	0.2361626082608552	0.5000000000000000
0.3399161564391449	0.3112571878502592	0.5000000000000000
0.7343126444704211	0.3114929015012322	0.5000000000000000
0.4413269882397657	0.4042096086461839	0.5000000000000000
0.6327285571624586	0.4043892959858582	0.5000000000000000
0.4410330184963414	0.6431458031931498	0.5000000000000000
0.6324561050586794	0.6431914900719775	0.5000000000000000
0.3396868097158148	0.7361578450737483	0.5000000000000000
0.7341127342999627	0.7361174086527527	0.5000000000000000
0.2343126430347198	0.8114904792305992	0.5000000000000000
0.8399178494417114	0.8112576626435555	0.5000000000000000
0.1327252805180308	0.9043948769906009	0.5000000000000000
0.9413273580116552	0.9042142995428577	0.5000000000000000
0.7848111101182482	0.0236098669572087	0.5000000000000000
0.2890201876080596	0.0239364855688038	0.5000000000000000
0.2848092919273171	0.5236087047319984	0.5000000000000000
0.7890232743246770	0.5239306049195065	0.5000000000000000

Ga-GD-Hex.

1.0000000000000000		
13.2503228556836792	0.0000000000000000	0.0000000000000000
6.6251614278418387	11.4751162013699908	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	Ga
12	2

Direct

0.4168211591972693	0.1663465669688975	0.5000000054087863
0.4705046454797071	0.0589776716865273	0.5000000022487967
0.4168250928640873	0.4168248954147842	0.5000000057090332
0.4705090270905643	0.4705101506542846	0.5000000017424000
0.5294878528397078	0.5294887678875213	0.5000000015687718
0.5831717445732139	0.5831735021044793	0.5000000047087312
0.5831685518761702	0.8336511215681313	0.4999999892466818
0.5294860254475822	0.9410198900390085	0.4999999960918800
0.1663466580220287	0.4168198796362290	0.5000000160412839
0.0589781916718906	0.4705039377429614	0.5000000023367903
0.8336518797702226	0.5831699183291832	0.4999999841034821
0.9410206790657654	0.5294866241615992	0.4999999907135262
0.3333313685768218	0.3333325302040393	0.5000000096051238
0.6666658567067998	0.6666647456955275	0.4999999904747554

Ga-GD-Rec.

1.000000000000000

16.6540885105193013 0.000000000000000 0.000000000000000

0.000000000000000 12.0675236196701299 0.000000000000000

0.000000000000000 0.000000000000000 20.000000000000000

C Ga

22 2

Direct

0.4218459260096168	0.4964931504194041	0.5000226827920358
0.4958275883804006	0.4964673349217605	0.5000215655362084
0.0789816888856620	0.9971833195339386	0.4999961682955529
0.5771315882547441	0.4965044390364071	0.5000390814215692
0.6511168935797969	0.4965294783132563	0.5000165716264604
0.8240185078533955	0.6347160811294970	0.4999989186032607
0.8646532021411488	0.7202284466412223	0.4999996698422322
0.9090358766711830	0.8134762995806426	0.4999993979899529
0.9502693973440230	0.8980086228857971	0.5000000787519525
0.8261751797291552	0.3622530321975574	0.5000056995849320
0.8665366662608065	0.2764663062768733	0.4999958325842186
0.9101749492265938	0.1824659221911773	0.4999757846075497
0.9505883193566333	0.0971483990462687	0.4999716135889685
0.9940118693868811	0.9974183528205529	0.4999870095017300
0.2488879649328339	0.6344038659796780	0.5000537980226483
0.2082087365176051	0.7198734413931192	0.5000362513688046
0.1637182643337454	0.8130076748342887	0.5000271810368204
0.1225292414691452	0.8975852398041013	0.5000059941804977
0.2467864883800530	0.3620569130227480	0.4999150117810913
0.2064376659872593	0.2762665040438606	0.4999714547946041
0.1628736325069511	0.1821933193276877	0.4999805720783712
0.1226359113741040	0.0967144473722783	0.4999819525359470
0.3068757714289490	0.4974282369611629	0.4999863457717311
0.7661045762914824	0.4976615479460094	0.5000138081594869

Ga-GY-Hex.

1.000000000000000		
8.7947210559296067	0.000000000000000	0.000000000000000
4.3973605279648016	7.6164518536298784	0.000000000000000
0.000000000000000	0.000000000000000	20.000000000000000

C Ga
6 2

Direct

0.4596574922302636	0.0806688379379565	0.4999999945189799
0.4596076288714670	0.4596033510928095	0.4999998958912002
0.5403132687911238	0.5403151394530994	0.4999998946785453
0.5403712724472527	0.9192522158431089	0.4999998966410928
0.0806694991404839	0.4596579110833829	0.5000002736979923
0.9192533362950002	0.5403727920773846	0.5000001307869013
0.3332976713742539	0.3332967404419165	0.5000003062133942
0.6666312440808682	0.6666345684811503	0.4999996075718585

Ga-GY-Rec.

1.000000000000000		
11.2015821655039396	0.000000000000000	0.000000000000000
0.000000000000000	7.7994668115346819	0.000000000000000
0.000000000000000	0.000000000000000	20.000000000000000

C Ga
12 2

Direct

0.4505644876204968	0.4989732516911403	0.4999976680634788
0.5603340009172157	0.4989110397850141	0.4999977891951275
0.8195793412323056	0.7095869489764652	0.4999985307655166
0.0684659713829987	0.9977183913590721	0.4999994435192008
0.8781826066088954	0.8425882929299675	0.4999988842436025
0.8193017075886289	0.2862557960404502	0.4999957111172577
0.8778843887770265	0.1532336699588939	0.4999888301208699
0.9432091143948398	0.9980011357412550	0.4999986185136933
0.1331991189264699	0.8420728971445115	0.5000051759803412
0.1914805243586315	0.7088347913533113	0.5000243159819604
0.1927867229558444	0.2854335655204494	0.4999980119019867
0.1339489524535082	0.1526854667638275	0.4999975500078477
0.2790942426861491	0.4976690263160890	0.5000039577133819
0.7319686540969670	0.4980357264195518	0.4999956318757199

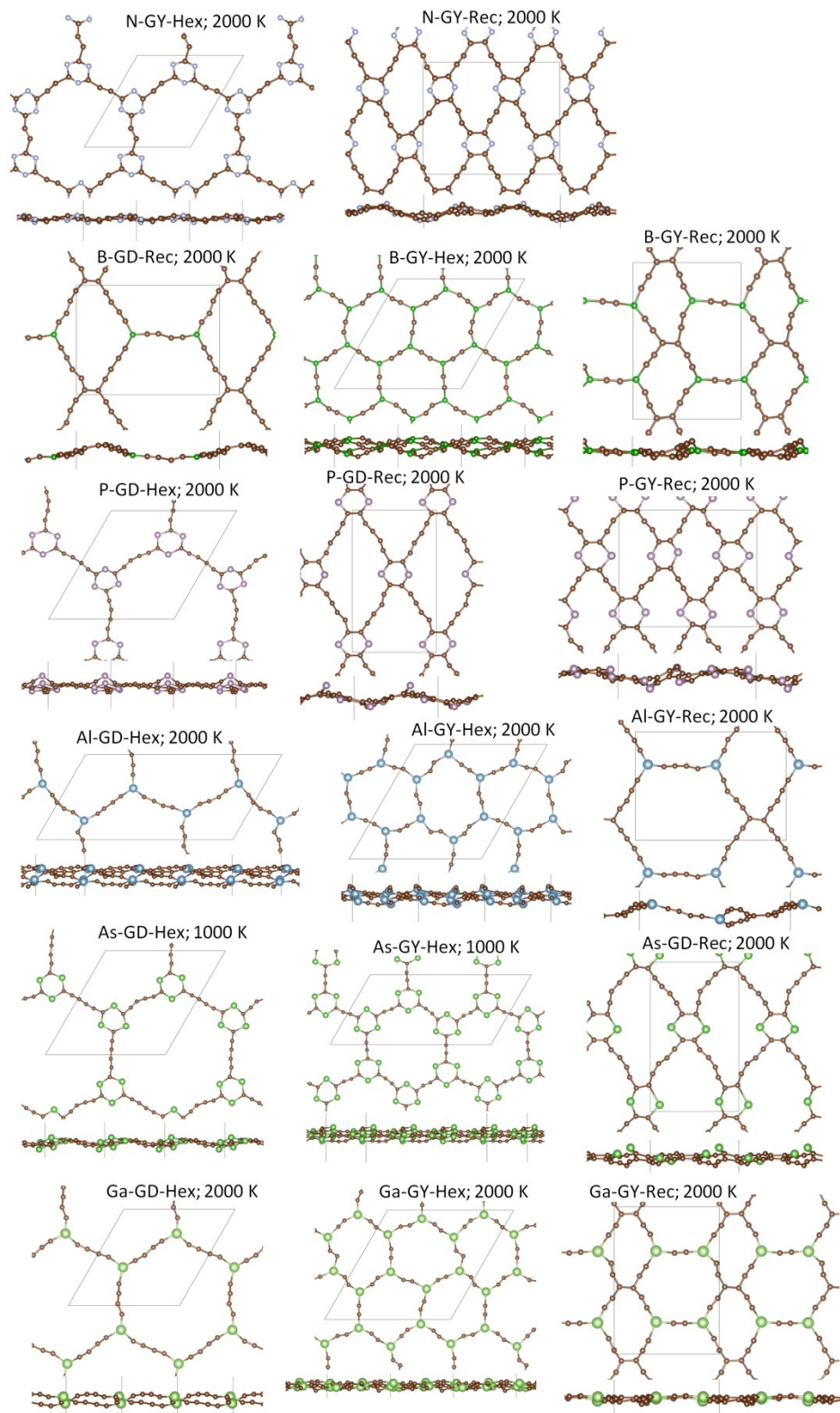


Fig. S1, Top and side views of predicted monolayers at different temperatures after the AIMD simulations for 20 ps. The black lines define the simulated systems.

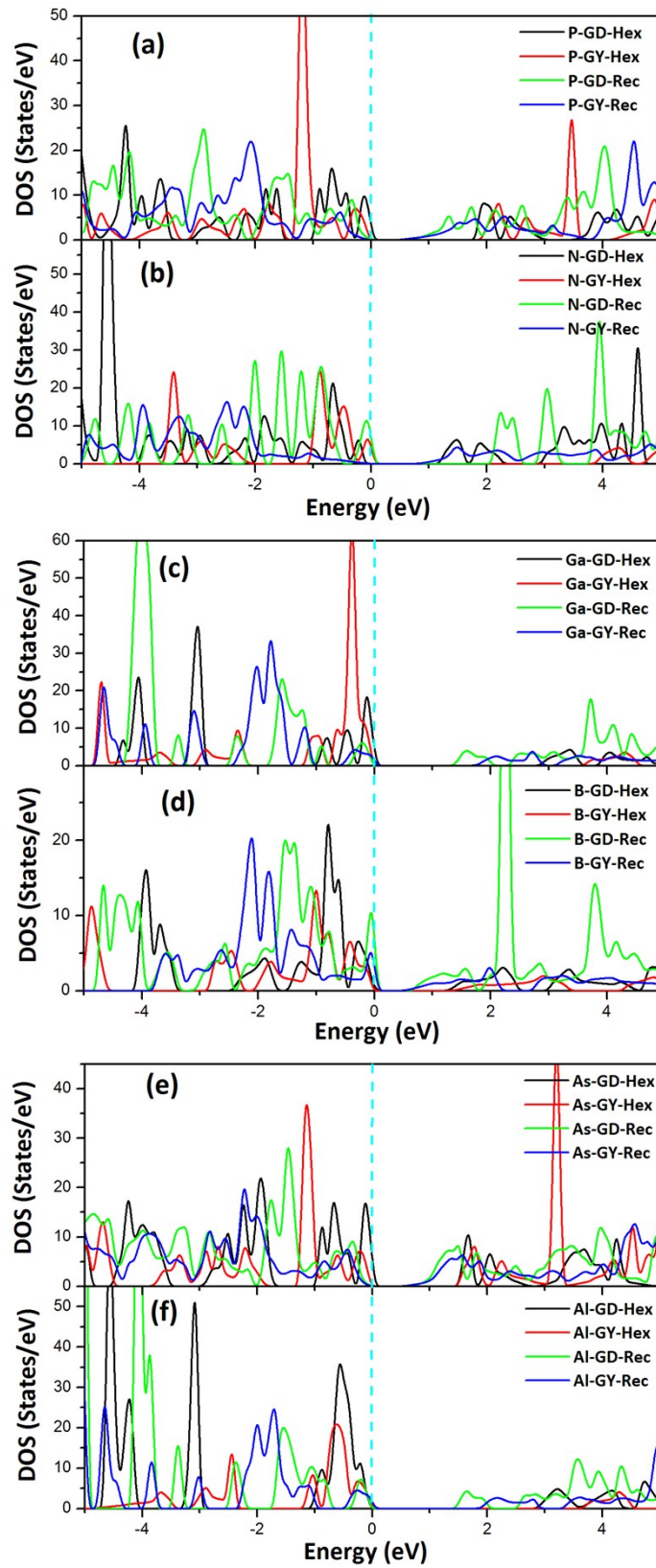


Fig. S2. Total electronic density of states predicted by the HSE06 functional. The Fermi energy is aligned to zero.