

**Extremely high tensile strength and superior thermal conductivity
of a sp³-hybridized superhard C₂₄ fullerene crystal.**

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1. Crystal structure of 3d-C₂₄.

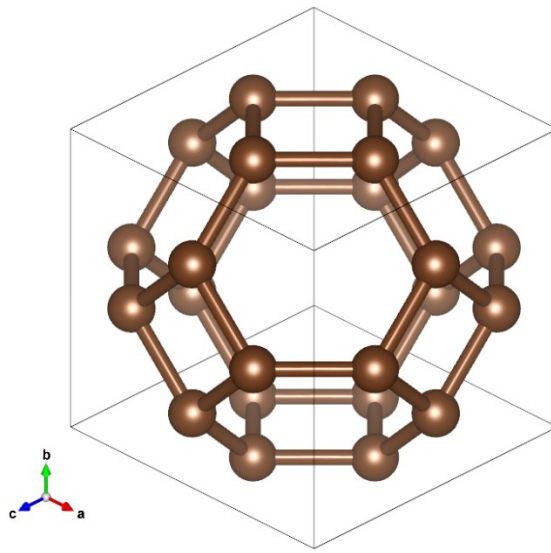


Fig. S1. Unit cell of the 3d-C₂₄ crystal.

2. A NVT *ab initio* molecular dynamics simulation is performed for the 3d-C₂₄ crystal at 2700 K. We find that the 3d-C₂₄ is still stable at high temperature.

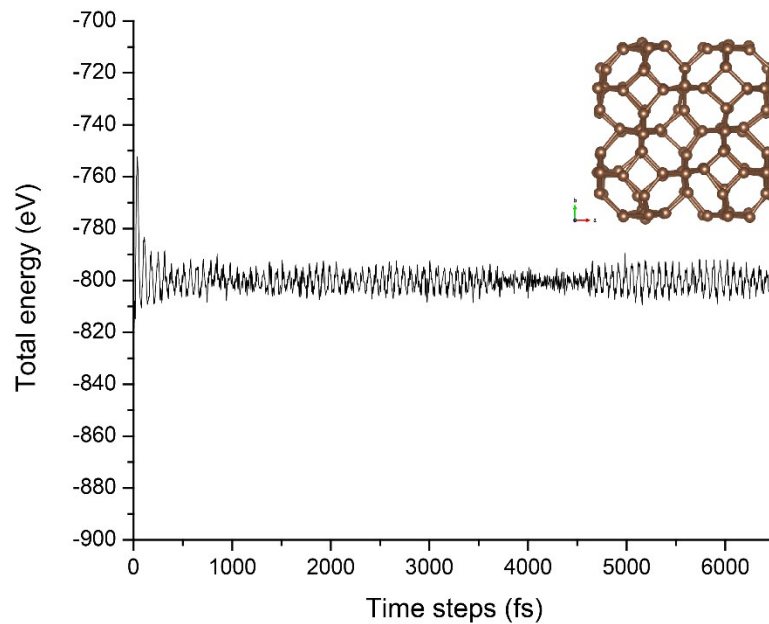


Fig. S2. Total energy change with time step within 6 ps for the 3d-C₂₄. The insert shows the 2×2×2 supercell of 3d-C₂₄ at 6 ps.

3. The details hardness calculations based on the models presented by Gao et al. and Šimůnek et al.

According to the model presented by Gao et al.,^[1] the hardness of 3d-C₂₄ is calculated by the formula of $H_v^{Gao} = 350 \left[\left(N_e^{2/3} \right)^{-1.191 f_i} / \left(d^{2.5} \right) \right]$ and is 80.9 GPa, where the N_e is the electron density, the d is the bond length, and f_i is the Phillips ionicity^[2].

According to the model presented by Šimůnek et al.,^[3] the hardness of 3d-C₂₄ is calculated by the formula of $H_v^{SV} = \frac{C}{\Omega} \sqrt{e_i e_i} / (d_{ii} n_{ii})$ and is 73.9 GPa, where the proportionality constant C is 1550, the Ω is the equilibrium volume, the e_i is 4.121 for carbon, the n_{ii} is the number of nearest neighbor bonds, and the d_{ii} is the bond length.

4. Structural parameters and atomic coordinates of 3d-C₂₄, Diamond, H-carbon, M-carbon, TC₈, T-carbon, Z-carbon, 3060-Carbon, Alpha-Carbon, bct carbon and Fullerite C₂₄ carbon allotropes with “VASP” format.

No.1 3d-C₂₄

3d-C₂₄

```

1. 0000000000000000
   4. 3710358478556905   0. 0000000000000000   0. 0000000000000000
   0. 0000000000000000   4. 3710358478556905   0. 0000000000000000
   0. 0000000000000000   0. 0000000000000000   4. 3710358478556905

```

C

12

Direct

```

0. 2500000000000000   0. 5000000000000000   0. 0000000000000000
0. 7500000000000000   0. 5000000000000000   0. 0000000000000000
0. 0000000000000000   0. 2500000000000000   0. 5000000000000000
0. 0000000000000000   0. 7500000000000000   0. 5000000000000000
0. 5000000000000000   0. 0000000000000000   0. 2500000000000000
0. 5000000000000000   0. 0000000000000000   0. 7500000000000000
0. 5000000000000000   0. 2500000000000000   0. 0000000000000000
0. 5000000000000000   0. 7500000000000000   0. 0000000000000000
0. 2500000000000000   0. 0000000000000000   0. 5000000000000000
0. 7500000000000000   0. 0000000000000000   0. 5000000000000000
0. 0000000000000000   0. 5000000000000000   0. 7500000000000000
0. 0000000000000000   0. 5000000000000000   0. 2500000000000000

```

No.2 Diamond

Diamond

1. 000000000000000

3. 5622356338059822	0. 0000000000000000	0. 0000000000000000
0. 0000000000000000	3. 5622356338059822	0. 0000000000000000
0. 0000000000000000	0. 0000000000000000	3. 5622356338059822

C

8

Direct

0. 0000000000000000	0. 0000000000000000	0. 0000000000000000
0. 0000000000000000	0. 5000000000000000	0. 5000000000000000
0. 5000000000000000	0. 0000000000000000	0. 5000000000000000
0. 5000000000000000	0. 5000000000000000	0. 0000000000000000
0. 7500000000000000	0. 2500000000000000	0. 7500000000000000
0. 2500000000000000	0. 2500000000000000	0. 2500000000000000
0. 2500000000000000	0. 7500000000000000	0. 7500000000000000
0. 7500000000000000	0. 7500000000000000	0. 2500000000000000

No.3 H-carbon

H-carbon

1. 000000000000000

9. 3380332994729454	0. 0000000000000000	-0. 0000248226775821
-4. 6690166497364727	8. 0866835269813109	0. 0000124113387910
0. 0000117514830986	0. 0000000000000000	4. 2303716978227879

C

36

Direct

0. 1577917046712827	0. 0000000000000000	0. 1848391607861188
0. 3037760285966300	0. 0000000000000000	0. 3365113301248783
0. 4342469287419490	0. 0000000000000000	0. 1670930921744898
0. 5657529043566072	0. 0000000000000000	0. 3315780340684142
0. 6962240103356265	0. 0000000000000000	0. 1621617476204165
0. 8422082722843811	0. 0000000000000000	0. 3138358672099599
0. 0000006814303646	0. 1577926685639781	0. 1848384347199499
0. 1577920229073726	0. 1577926975101320	0. 3138367521081733
0. 0000038297588674	0. 3037759131582760	0. 3365119666802912
0. 3037720564440178	0. 3037758939127286	0. 1621615679850450
0. 0000017215278092	0. 4342456665324974	0. 1670928202808142
0. 4342440860429022	0. 4342458574597785	0. 3315788713558234
0. 9999982025831287	0. 5657540895402207	0. 3315788713558234

0. 5657560289953167	0. 5657542804675018	0. 1670928202808142
0. 9999961505312811	0. 6962240830872730	0. 1621615679850450
0. 6962279046005975	0. 6962240638417256	0. 3365119666802912
0. 9999993133972325	0. 8422072644898719	0. 3138367521081733
0. 8422079868663914	0. 8422072934360259	0. 1848384347199499
0. 1577917183639599	0. 0000000000000000	0. 81383600000000660
0. 3037759348396634	0. 0000000000000000	0. 6621620721689538
0. 4342471013350320	0. 0000000000000000	0. 8315781763772776
0. 5657530358519622	0. 0000000000000000	0. 6670929655932909
0. 6962240191636297	0. 0000000000000000	0. 8365110143116752
0. 8422083264034299	0. 0000000000000000	0. 6848390211918982
0. 0000007054998363	0. 1577927060113780	0. 8138367438104694
0. 1577919858248009	0. 1577926762326953	0. 6848384410370016
0. 0000038462954350	0. 3037758499861596	0. 6621616248826854
0. 3037720665778636	0. 3037759018344701	0. 8365119076593572
0. 0000017957287142	0. 4342458608014326	0. 8315789150067801
0. 4342439246366325	0. 4342457622898692	0. 6670927856599107
0. 9999981363467683	0. 5657541847101299	0. 6670927856599107
0. 5657559089272794	0. 5657540861985666	0. 8315789150067801
0. 9999961527433925	0. 6962240751655315	0. 8365119076593572
0. 6962279843092674	0. 6962241270138421	0. 6621616248826854
0. 9999992975921046	0. 8422072857673086	0. 6848384410370016
0. 8422079734884633	0. 8422072559886260	0. 8138367438104694

No.4 M-carbon

M-carbon

1. 0000000000000000

9. 1613708068335207 0. 0000000000000000 -0. 0031144906245932

0. 0000000000000000 2. 5172851769501636 0. 0000000000000000

-0. 5026654345872984 0. 0000000000000000 4. 1074387431602775

C

16

Direct

0. 4427600186756848 0. 5000000000000000 0. 1205098076507767

0. 5572399613243135 0. 5000000000000000 0. 8794901983492238

0. 9427599926756827 0. 0000000000000000 0. 1205098076507767

0. 0572399873243157 0. 0000000000000000 0. 8794901983492238

0. 2857348143075242 0. 5000000000000000 0. 9407466653062571

0.7142652446924771	0.5000000000000000	0.0592533326937428
0.7857347613075234	0.0000000000000000	0.9407466653062571
0.2142651916924763	0.0000000000000000	0.0592533326937428
0.2713518678199733	0.0000000000000000	0.4146582179855187
0.7286481661800295	0.0000000000000000	0.5853418020144829
0.7713518408199675	0.5000000000000000	0.4146582179855187
0.2286481401800273	0.5000000000000000	0.5853418020144829
0.4418239828730322	0.0000000000000000	0.3463970551059248
0.5581760231269683	0.0000000000000000	0.6536029358940709
0.9418240348730293	0.5000000000000000	0.3463970551059248
0.0581759901269692	0.5000000000000000	0.6536029358940709

No.5 TC₈

TC₈

1.0000000000000000		
4.4173692119152363	0.0000000000000000	0.0000000000000000
0.0000000000000000	4.4173692119152363	0.0000000000000000
0.0000000000000000	0.0000000000000000	3.4263040695818665

C

8

Direct

0.5000000000000000	0.0000000000000000	0.1946098064617132
0.5000000000000000	0.0000000000000000	0.8053901935382868
0.0000000000000000	0.5000000000000000	0.1946098064617132
0.0000000000000000	0.5000000000000000	0.8053901935382868
0.2520953277431559	0.0000000000000000	0.5000000000000000
0.7479046722568441	0.0000000000000000	0.5000000000000000
0.0000000000000000	0.2520953277431559	0.5000000000000000
0.0000000000000000	0.7479046722568441	0.5000000000000000

No.6 T-carbon

T-carbon

1.0000000000000000		
7.4931403931078311	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.4931403931078311	0.0000000000000000
0.0000000000000000	0.0000000000000000	7.4931403931078311

C

32

Direct

0. 0706395167053770	0. 0706395167053770	0. 0706395167053770
0. 9293604362946226	0. 4293604992946243	0. 5706395327053784
0. 4293604992946243	0. 5706395327053784	0. 9293604362946226
0. 5706395327053784	0. 9293604362946226	0. 4293604992946243
0. 8206395477053761	0. 3206395167053770	0. 6793604832946230
0. 1793604832946230	0. 1793604832946230	0. 1793604832946230
0. 3206395167053770	0. 6793604832946230	0. 8206395477053761
0. 6793604832946230	0. 8206395477053761	0. 3206395167053770
0. 3206395167053770	0. 8206395477053761	0. 6793604832946230
0. 8206395477053761	0. 6793604832946230	0. 3206395167053770
0. 6793604832946230	0. 3206395167053770	0. 8206395477053761
0. 4293604992946243	0. 9293604362946226	0. 5706395327053784
0. 9293604362946226	0. 5706395327053784	0. 4293604992946243
0. 5706395327053784	0. 4293604992946243	0. 9293604362946226
0. 0706395167053770	0. 5706395327053784	0. 5706395327053784
0. 9293604362946226	0. 9293604362946226	0. 0706395167053770
0. 4293604992946243	0. 0706395167053770	0. 4293604992946243
0. 8206395477053761	0. 8206395477053761	0. 1793604832946230
0. 1793604832946230	0. 6793604832946230	0. 6793604832946230
0. 3206395167053770	0. 1793604832946230	0. 3206395167053770
0. 3206395167053770	0. 3206395167053770	0. 1793604832946230
0. 8206395477053761	0. 1793604832946230	0. 8206395477053761
0. 4293604992946243	0. 4293604992946243	0. 0706395167053770
0. 9293604362946226	0. 0706395167053770	0. 9293604362946226
0. 5706395327053784	0. 0706395167053770	0. 5706395327053784
0. 0706395167053770	0. 9293604362946226	0. 9293604362946226
0. 6793604832946230	0. 1793604832946230	0. 6793604832946230
0. 1793604832946230	0. 8206395477053761	0. 8206395477053761
0. 1793604832946230	0. 3206395167053770	0. 3206395167053770
0. 0706395167053770	0. 4293604992946243	0. 4293604992946243
0. 5706395327053784	0. 5706395327053784	0. 0706395167053770
0. 6793604832946230	0. 6793604832946230	0. 1793604832946230

No.7 Z-carbon

Z-carbon

1. 00000000000000

8. 7425123485473097	0. 0000000000000000	0. 0000000000000000
0. 0000000000000000	4. 2414525143014004	0. 0000000000000000
0. 0000000000000000	0. 0000000000000000	2. 5072149370721957

C

16

Direct

0. 3333756112993598	0. 3148926936312719	0. 0000000000000000
0. 6666243887006402	0. 6851073343687304	0. 0000000000000000
0. 6666243887006402	0. 3148926936312719	0. 0000000000000000
0. 3333756112993598	0. 6851073343687304	0. 0000000000000000
0. 8333756112993598	0. 8148926656312696	0. 0000000000000000
0. 1666243887006402	0. 1851073203687292	0. 0000000000000000
0. 1666243887006402	0. 8148926656312696	0. 0000000000000000
0. 8333756112993598	0. 1851073203687292	0. 0000000000000000
0. 0891964046896803	0. 3154426682293163	0. 5000000000000000
0. 9108036023103239	0. 6845573597706860	0. 5000000000000000
0. 9108036023103239	0. 3154426682293163	0. 5000000000000000
0. 0891964046896803	0. 6845573597706860	0. 5000000000000000
0. 5891963976896761	0. 8154426402293140	0. 5000000000000000
0. 4108036023103239	0. 1845573457706848	0. 5000000000000000
0. 4108036023103239	0. 8154426402293140	0. 5000000000000000
0. 5891963976896761	0. 1845573457706848	0. 5000000000000000

No.8 3060-Carbon

3060-Carbon

1. 0000000000000000

9. 3503357536334732	0. 0000000000000000	0. 0000000000000000
-4. 6751678768167366	8. 0976282965605044	0. 0000000000000000
0. 0000000000000000	0. 0000000000000000	4. 3851736481951731

C

48

Direct

0. 2389919553026871	0. 3229932174546519	0. 1138482335069924
0. 3229932174546803	0. 2389919553026729	0. 6138482185069876
0. 3229931633285616	0. 2389919140300023	0. 9703308765331471
0. 9159988965166121	0. 2389908883110365	0. 1138495385763250
0. 2389919140300236	0. 3229931633285332	0. 4703309065331567
0. 0840012057751309	0. 3229927231417378	0. 6138484099342989
0. 0840013594578721	0. 3229927022917991	0. 9703313607519419

0. 6770072468582242	0. 9159987872248578	0. 1138484249343037
0. 9159990440381520	0. 2389911055099816	0. 4703316803187150
0. 7610091416889233	0. 0840010964833624	0. 6138495235763202
0. 7610089244899712	0. 0840009489618225	0. 9703316503187125
0. 7610080746973154	0. 6770067525453527	0. 1138482335069924
0. 6770072677081558	0. 9159986335421166	0. 4703313907519444
0. 6770067525453243	0. 7610080746973296	0. 6138482185069876
0. 6770068066714501	0. 7610081159700002	0. 9703308765331471
0. 0840010964833908	0. 7610091416889659	0. 1138495385763250
0. 7610081159699789	0. 6770068066714714	0. 4703309065331567
0. 9159987872248720	0. 6770072468582669	0. 6138484099342989
0. 9159986335421308	0. 6770072677081984	0. 9703313607519419
0. 3229927231417804	0. 0840012057751451	0. 1138484249343037
0. 0840009489618510	0. 7610089244900209	0. 4703316803187150
0. 2389908883110792	0. 9159988965166406	0. 6138495235763202
0. 2389911055100242	0. 9159990440381804	0. 9703316503187125
0. 3229927022918488	0. 0840013594578863	0. 4703313907519444
0. 3349611156243952	0. 5186331267044366	0. 1149599371727561
0. 3349608880485135	0. 5186331935800226	0. 4692199216121651
0. 4813668732955492	0. 6650389133755752	0. 6149599521727538
0. 4813668064199632	0. 6650391409514640	0. 9692199216121651
0. 4813667802063506	0. 8163280743559227	0. 1149601212553364
0. 4813669311987425	0. 8163283022408763	0. 4692203292896409
0. 3349606401266385	0. 8163281586853444	0. 6149600791063747
0. 3349607935023897	0. 8163282257593423	0. 9692195239423285
0. 1836718263146722	0. 6650393888733532	0. 1149600641063770
0. 1836717592406671	0. 6650392354975949	0. 4692195239423285
0. 1836719106440938	0. 5186332197936565	0. 6149601362553412
0. 1836716827591403	0. 5186330688012646	0. 9692203292896409
0. 5186332197936494	0. 1836719106440725	0. 1149601212553364
0. 5186330688012504	0. 1836716827591189	0. 4692203292896409
0. 6650393888733603	0. 1836718263146508	0. 6149600791063747
0. 6650392354976091	0. 1836717592406529	0. 9692195239423285
0. 8163281586853230	0. 3349606401266456	0. 1149600641063770
0. 8163282257593281	0. 3349607935024039	0. 4692195239423285
0. 8163280743559014	0. 4813667802063435	0. 6149601362553412
0. 8163283022408550	0. 4813669311987354	0. 9692203292896409
0. 6650389133756036	0. 4813668732955634	0. 1149599371727561
0. 6650391409514853	0. 4813668064199774	0. 4692199216121651
0. 5186331267044508	0. 3349611156244237	0. 6149599521727538
0. 5186331935800368	0. 3349608880485349	0. 9692199216121651

No.9 Alpha-Carbon

Alpha-Carbon

1. 000000000000000		
6. 1093850730928327	0. 0000000000001568	0. 0000000000000000
-3. 0546925365961459	5. 2908826748031066	0. 0000000000000000
0. 0000000000000000	0. 0000000000000000	2. 5446637376136683

C

12

Direct

0. 4085196697848517	0. 3266979637094423	0. 2500000000000000
0. 5914803302151483	0. 6733020362905577	0. 7500000000000000
0. 6733020362905577	0. 0818217070754201	0. 2500000000000000
0. 3266979637094423	0. 9181782929245799	0. 7500000000000000
0. 9181782929245799	0. 5914803302151483	0. 2500000000000000
0. 0818217070754201	0. 4085196697848517	0. 7500000000000000
0. 3266979637094423	0. 4085196697848517	0. 7500000000000000
0. 6733020362905577	0. 5914803302151483	0. 2500000000000000
0. 0818217070754201	0. 6733020362905577	0. 7500000000000000
0. 9181782929245799	0. 3266979637094423	0. 2500000000000000
0. 5914803302151483	0. 9181782929245799	0. 7500000000000000
0. 4085196697848517	0. 0818217070754201	0. 2500000000000000

No.10 bct carbon

bct carbon

1. 000000000000000		
4. 3661184814644871	0. 0000000000000000	0. 0000000000000000
0. 0000000000000000	4. 3661184814644871	0. 0000000000000000
0. 0000000000000000	0. 0000000000000000	2. 5046814060140683

C

8

Direct

0. 1802675203386528	0. 1802675203386528	0. 0000000000000000
0. 8197324526613485	0. 8197324526613485	0. 0000000000000000
0. 8197324526613485	0. 1802675203386528	0. 0000000000000000
0. 1802675203386528	0. 8197324526613485	0. 0000000000000000

0. 6802675473386515	0. 6802675473386515	0. 5000000000000000
0. 3197324796613472	0. 3197324796613472	0. 5000000000000000
0. 3197324796613472	0. 6802675473386515	0. 5000000000000000
0. 6802675473386515	0. 3197324796613472	0. 5000000000000000

No.11 Fullerite C₂₄

Fullerite C₂₄

1. 0000000000000000		
5. 9018979674869065	0. 0000000000000000	-0. 0000000000000000
-0. 0000000000000000	5. 9018979674869065	0. 0000000000000000
0. 0000000000000000	0. 0000000000000000	5. 9018979674869065

C

24

Direct

0. 6328426931980673	0. 0000000000000000	0. 8092412897394546
0. 3671573068019328	0. 0000000000000000	0. 1907587102605456
0. 3671573068019328	0. 0000000000000000	0. 8092412897394546
0. 6328426931980673	0. 0000000000000000	0. 1907587102605456
0. 8092412897394546	0. 6328426931980673	0. 0000000000000000
0. 1907587102605456	0. 3671573068019328	0. 0000000000000000
0. 8092412897394546	0. 3671573068019328	0. 0000000000000000
0. 1907587102605456	0. 6328426931980673	0. 0000000000000000
0. 0000000000000000	0. 8092412897394546	0. 6328426931980673
0. 0000000000000000	0. 1907587102605456	0. 3671573068019328
0. 0000000000000000	0. 8092412897394546	0. 3671573068019328
0. 0000000000000000	0. 1907587102605456	0. 6328426931980673
0. 0000000000000000	0. 6328426931980673	0. 1907587102605456
0. 0000000000000000	0. 3671573068019328	0. 8092412897394546
0. 0000000000000000	0. 3671573068019328	0. 1907587102605456
0. 0000000000000000	0. 6328426931980673	0. 8092412897394546
0. 6328426931980673	0. 8092412897394546	0. 0000000000000000
0. 3671573068019328	0. 1907587102605456	0. 0000000000000000
0. 3671573068019328	0. 8092412897394546	0. 0000000000000000
0. 6328426931980673	0. 1907587102605456	0. 0000000000000000
0. 8092412897394546	0. 0000000000000000	0. 3671573068019328
0. 1907587102605456	0. 0000000000000000	0. 6328426931980673
0. 8092412897394546	0. 0000000000000000	0. 6328426931980673
0. 1907587102605456	0. 0000000000000000	0. 3671573068019328

References

- [1] F. Gao, J. He, E. Wu, S. Liu, D. Yu, D. Li, S. Zhang and Y. Tian, *Phys. Rev. Lett.*, 2003, **91**, 015502.
- [2] J. C. Phillips, *Rev. Mod. Phys.*, 1970, **42**, 317–356.
- [3] A. Šimůnek and J. Vackář, *Phys. Rev. Lett.*, 2006, **96**, 085501.