

Supporting Information for

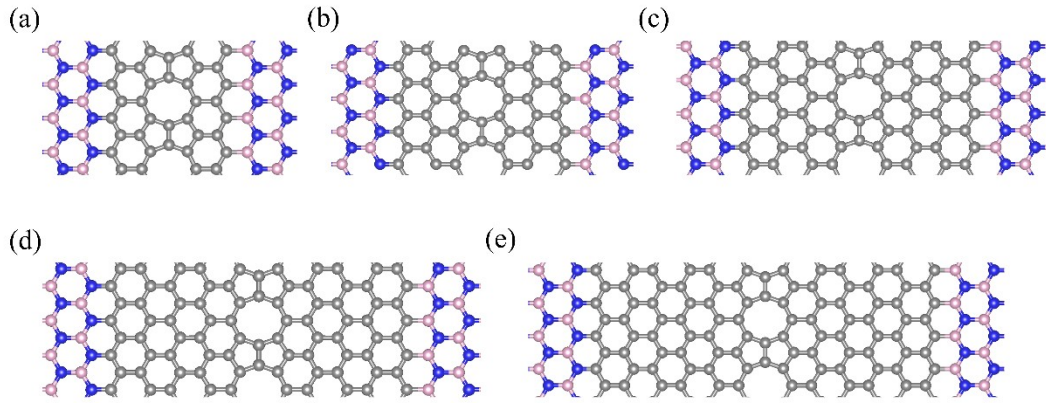
**Field-Free Control of Magnetism and Electronic States in  
ZGNR/h-BN Heterojunctions via Topological Line Defects**

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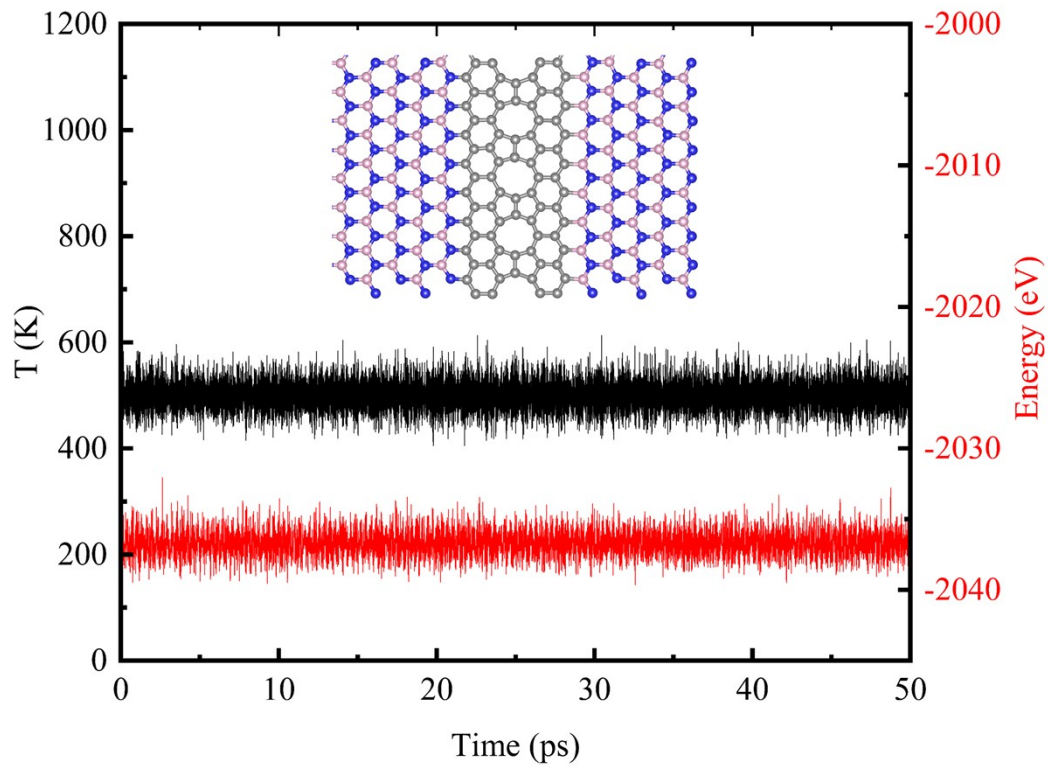
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Email: weiliu@zafu.edu.cn

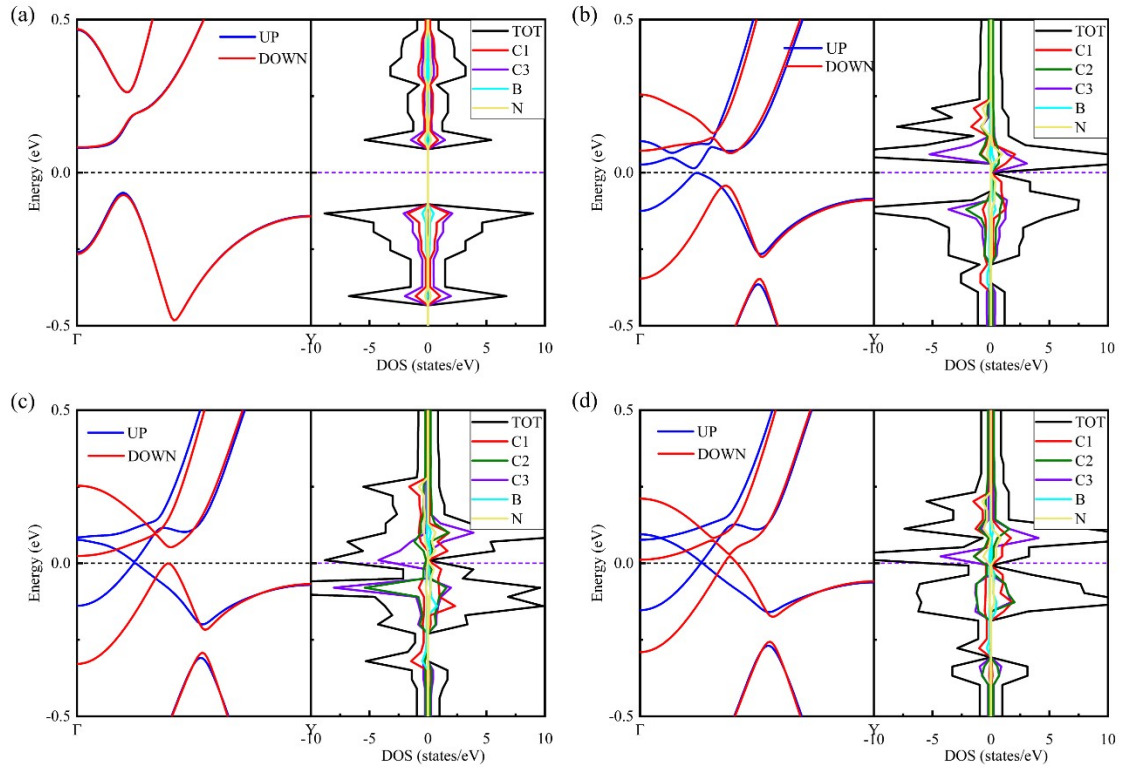
Keywords: graphene nanoribbons, half-semimetallicity, antiferromagnetism,  
ferrimagnetic, spintronics.



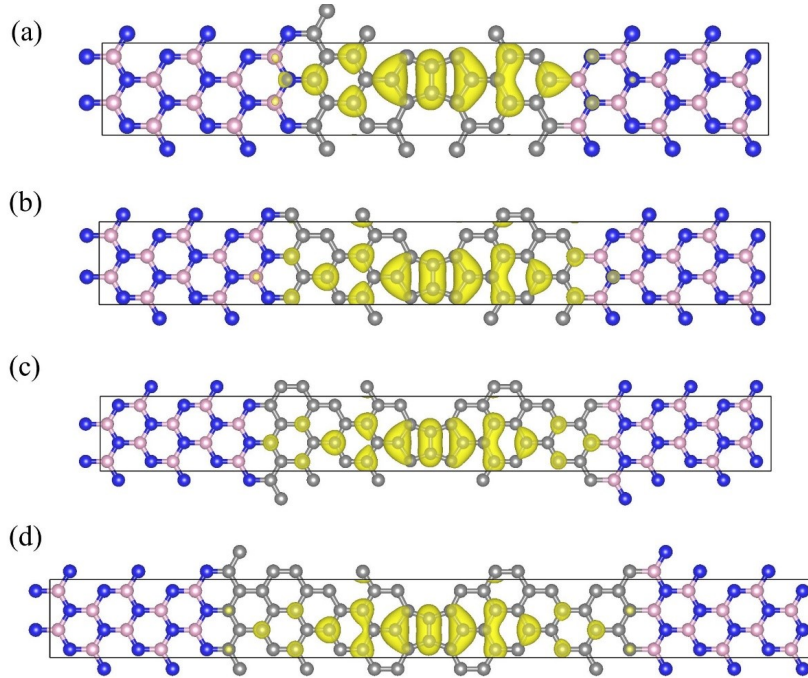
**FIG. S1.** Atomic structures of (a) ZGNR(558)/hBN-5, (b) ZGNR(558)/hBN-7, (c) ZGNR(558)/hBN-9, (d) ZGNR(558)/hBN-11, and (e) ZGNR(558)/hBN-13.



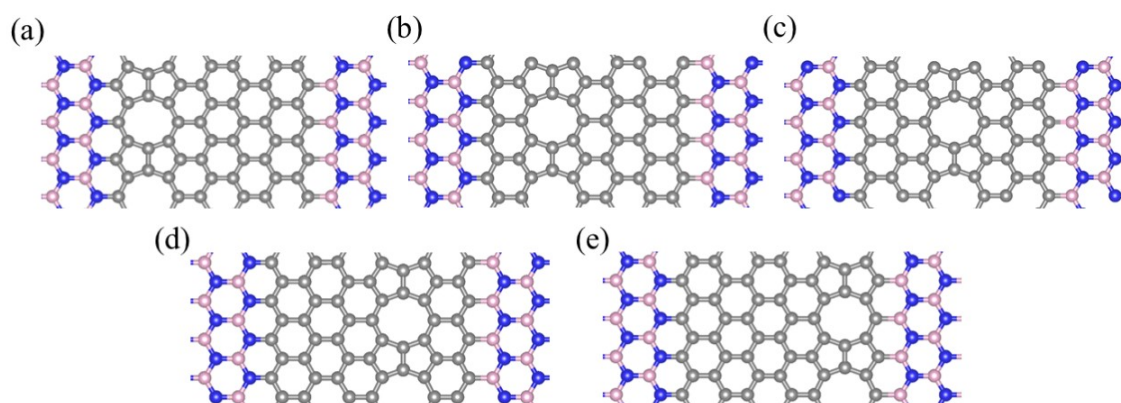
**FIG. S2.** Variations in simulated energy and temperature during the AIMD simulations of ZGNR(558)/hBN-5 over 50 ps with a time step of 1 fs.



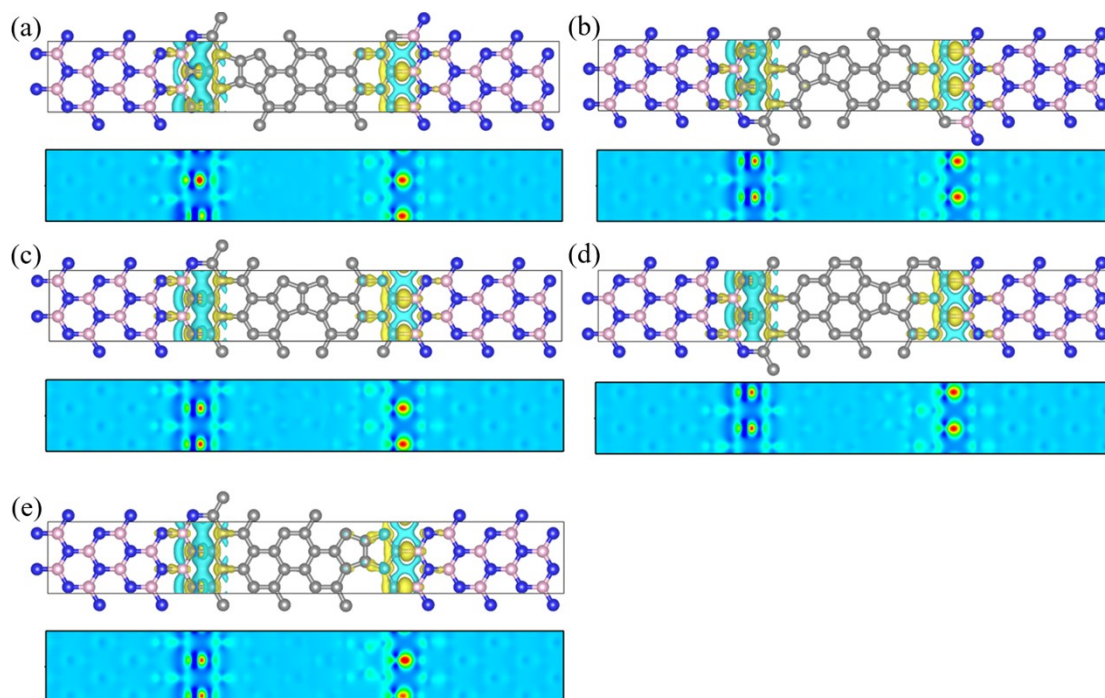
**FIG. S3.** Band structures and projected density of states of (a) ZGNR(558)/hBN-5, (b) ZGNR(558)/hBN-9, (c) ZGNR(558)/hBN-11, and (d) ZGNR(558)/hBN-13.



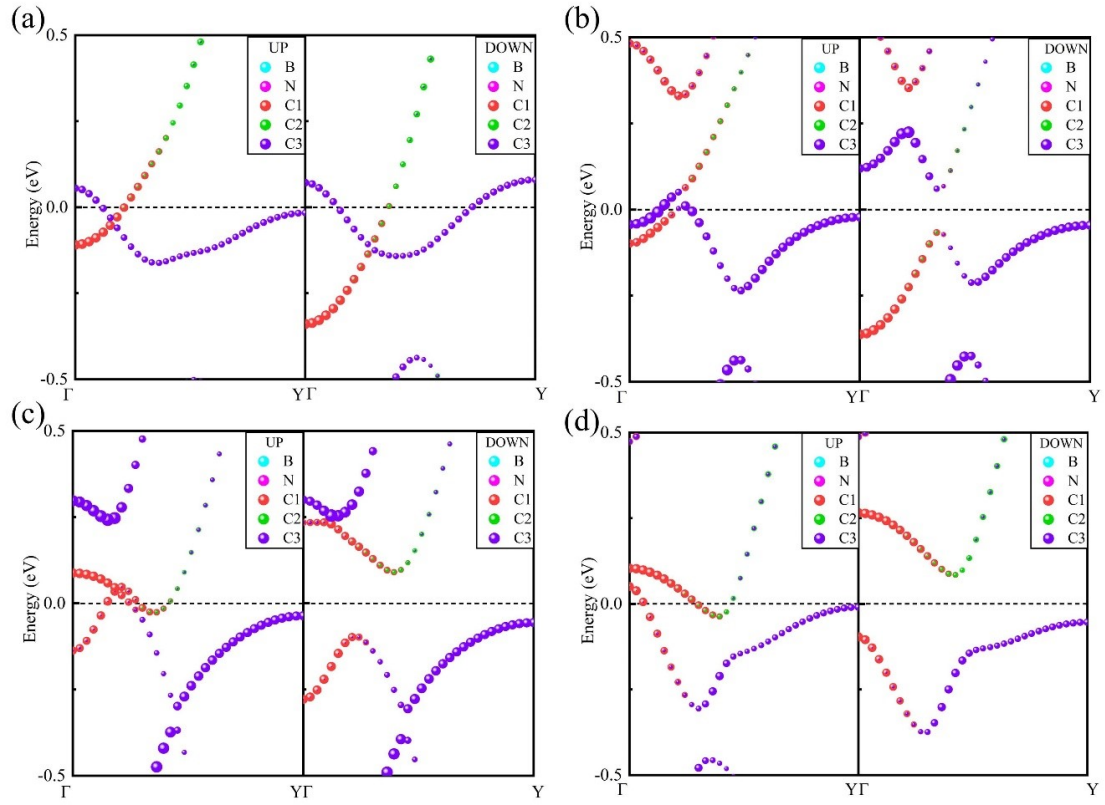
**FIG. S4.** Partial charge density near the Fermi level for (a) ZGNR(558)/hBN-7, (b) ZGNR(558)/hBN-9, (c) ZGNR(558)/hBN-11, and (d) ZGNR(558)/hBN-13.



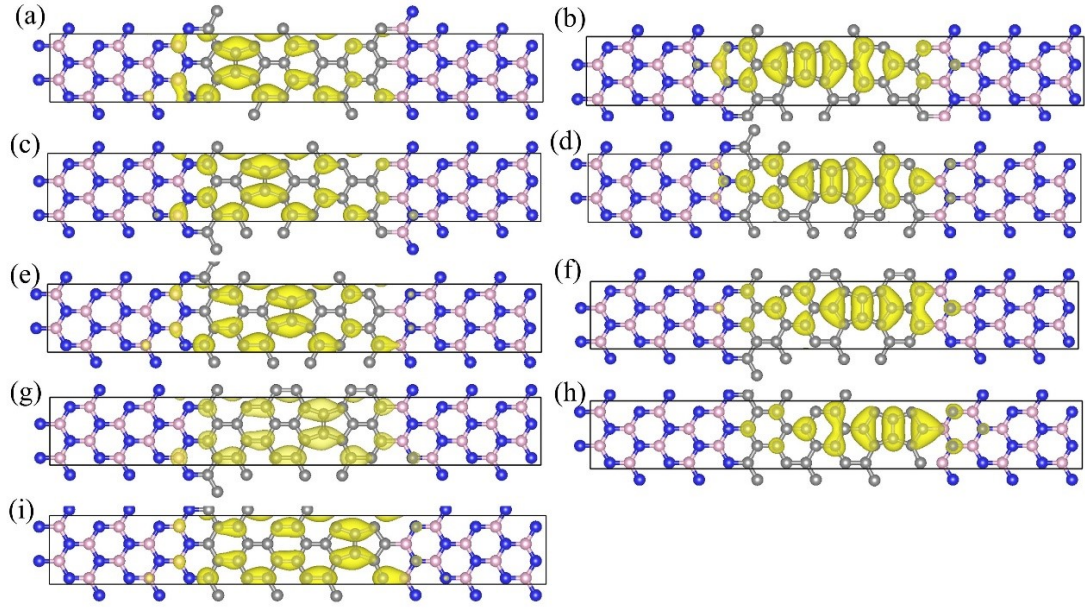
**FIG. S5.** Atomic structures of (a) ZGNR(558)/hBN-7(04), (b) ZGNR(558)/hBN-7(13), (c) ZGNR(558)/hBN-7(22), (d) ZGNR(558)/hBN-7(31), and (e) ZGNR(558)/hBN-7(40).



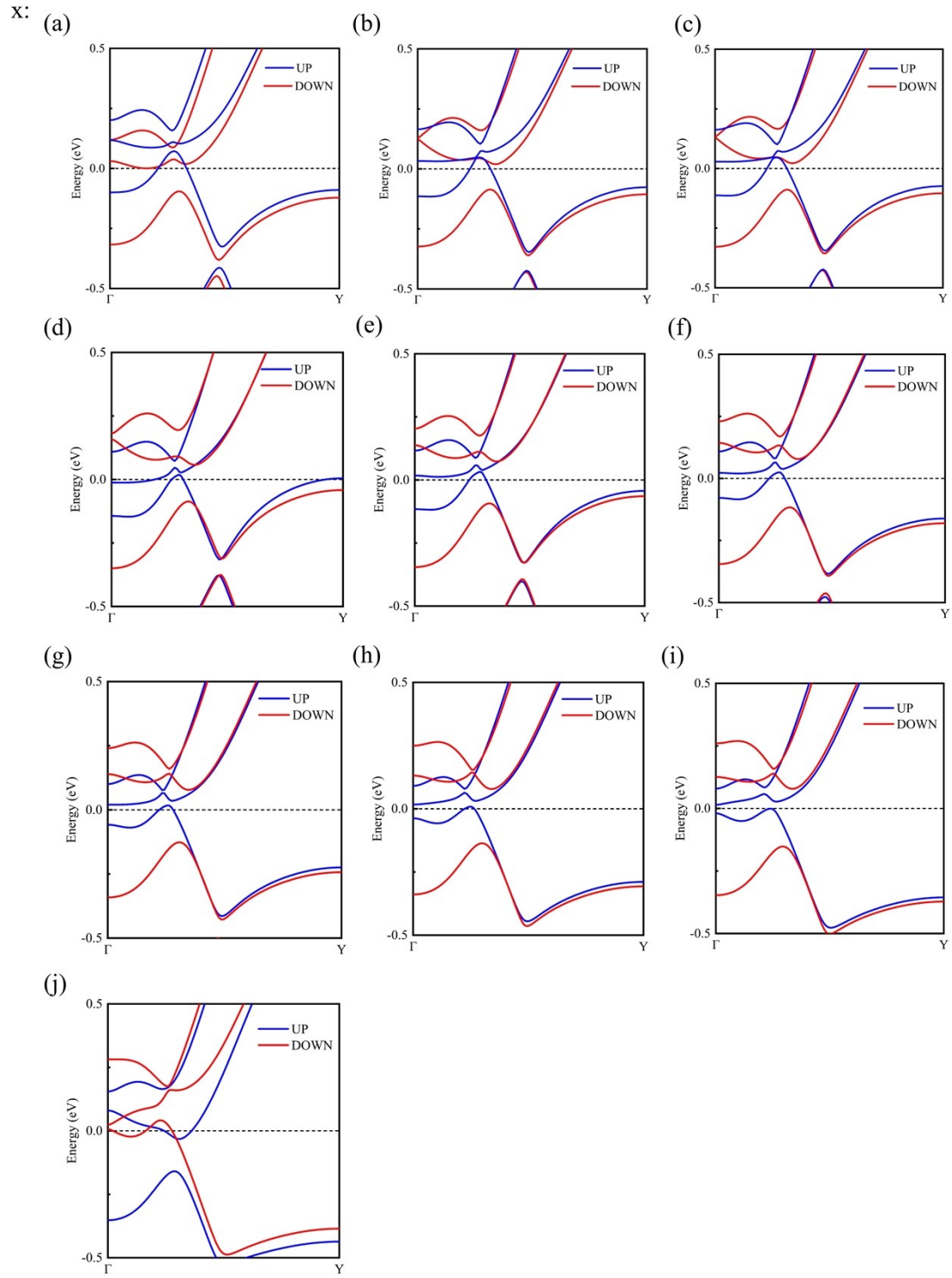
**FIG. S6.** The charge density difference distributions (top) and corresponding two-dimensional contour maps for (a) ZGNR(558)/hBN-7(04), (b) ZGNR(558)/hBN-7(13), (c) ZGNR(558)/hBN-7(22), (d) ZGNR(558)/hBN-7(31), and (e) ZGNR(558)/hBN-7(40).



**FIG. S7.** Projected band structures for (a) ZGNR(558)/hBN-7(04), (b) ZGNR(558)/hBN-7(13), (c) ZGNR(558)/hBN-7(31), and (d) ZGNR(558)/hBN-7(40).

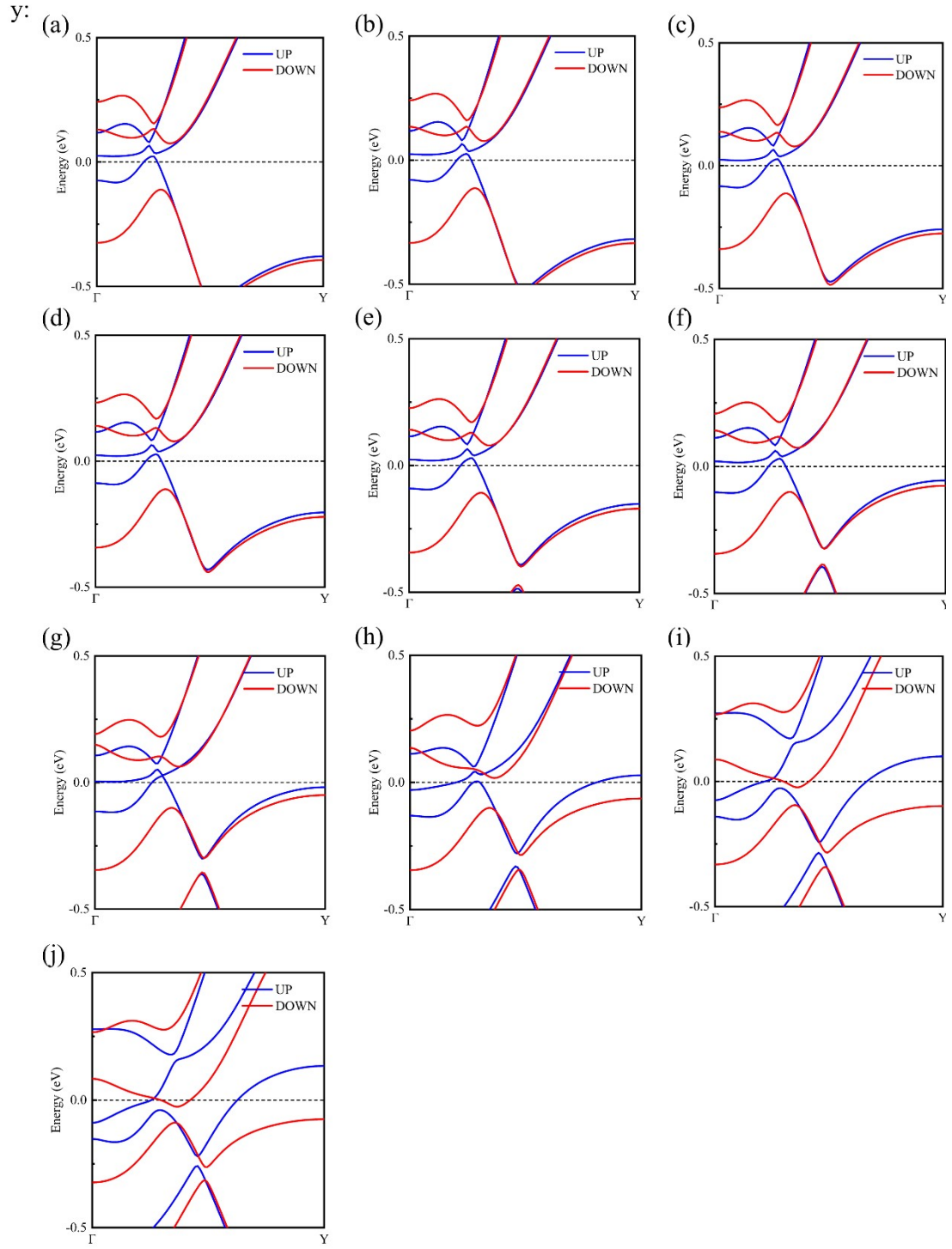


**FIG. S8.** (a) Partial charge density near the fermi level of ZGNR(558)/hBN-7(04). Partial charge density distributions at the (b) VBM and (c) CBM for ZGNR(558)/hBN-7(13). Partial charge density distributions at the (d) VBM and (e) CBM for ZGNR(558)/hBN-7(22). Partial charge density distributions at the (f) VBM and (g) CBM for ZGNR(558)/hBN-7(31). Partial charge density distributions at the (h) VBM and (i) CBM for ZGNR(558)/hBN-7(40).

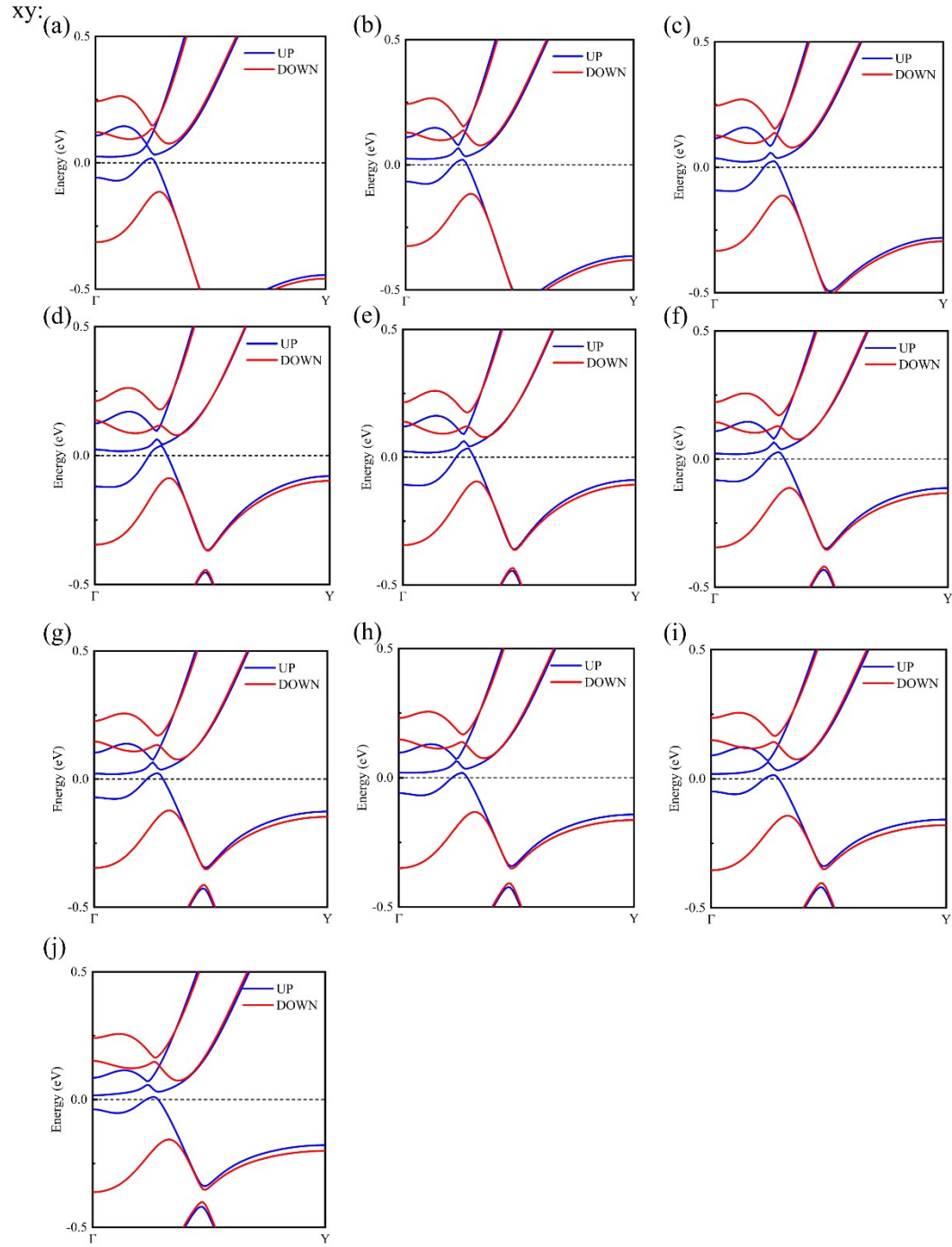


**F**

**IG. S9.** Band structures of ZGNR(558)/hBN-7 under uniaxial strain along the x-direction: (a)-(j) correspond to different distortion degrees (from -5% to 5%).



**FIG. S10.** Band structures of ZGNR(558)/hBN-7 under uniaxial strain along the y-direction: (a)-(j) correspond to different distortion degrees (from -5% to 5%).



**FIG. S11.** Band structures of ZGNR(558)/hBN-7 under biaxial strain: (a)-(j) correspond to different distortion degrees (from -5% to 5%).

**Table S1.** The binding energies of ZGNR/hBN-W, ZGNR(558)/hBN-W and ZGNR(558)/hBN-7 (LR).

Structure	$\Delta E$ (eV)	Structure	$\Delta E$ (eV)	Structure	$\Delta E$ (eV)
ZGNR/hBN-4	0.051	ZGNR(558)/hBN-5	0.045	ZGNR(558)/hBN-7(04)	0.039
ZGNR/hBN-6	0.047	ZGNR(558)/hBN-7	0.042	ZGNR(558)/hBN-7(13)	0.041
ZGNR/hBN-8	0.043	ZGNR(558)/hBN-9	0.040	ZGNR(558)/hBN-7(22)	0.042
ZGNR/hBN-10	0.039	ZGNR(558)/hBN-11	0.037	ZGNR(558)/hBN-7(31)	0.043
ZGNR/hBN-12	0.036	ZGNR(558)/hBN-13	0.035	ZGNR(558)/hBN-7(40)	0.042

**S2.**

Structure	mag ( $\mu B$ )	Structure	mag ( $\mu B$ )
ZGNR(558)/hBN-5	0	ZGNR(558)/hBN-7(04)	0.50
ZGNR(558)/hBN-7	0.0024	ZGNR(558)/hBN-7(13)	0.0115
ZGNR(558)/hBN-9	0.0091	ZGNR(558)/hBN-7(22)	0.0024
ZGNR(558)/hBN-11	0.064	ZGNR(558)/hBN-7(31)	0.0059
ZGNR(558)/hBN-13	0.077	ZGNR(558)/hBN-7(40)	0.0038

**Table**  
Total

magnetic moments of ZGNR(558)/hBN-W, and ZGNR(558)/hBN-7 (LR).

**The coordinates and unit cells for all the ZGNR/h-BN heterojunctions considered in the manuscript have been presented in CIF format as following:**

ZGNR/hBN-6

```

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_cell_length_b                 2.491333
_cell_length_c                 20.000000
_cell_angle_alpha              90.000000
_cell_angle_beta               90.000000
_cell_angle_gamma              90.000000
_cell_volume                   1728.559190
_space_group_name_H-M_alt      'P 1'
_space_group_IT_number         1

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_space_group_symop_operation_xyz
  'x, y, z'

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  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
  N1          1.0    0.043368    0.215634    0.164787    Biso  1.000000  N
  N2          1.0    0.106191    0.715762    0.164747    Biso  1.000000  N
  N3          1.0    0.169009    0.215892    0.164789    Biso  1.000000  N
  N4          1.0    0.231815    0.715916    0.164971    Biso  1.000000  N
  N5          1.0    0.729245    0.715680    0.165206    Biso  1.000000  N
  N6          1.0    0.792131    0.215746    0.164989    Biso  1.000000  N
  N7          1.0    0.854934    0.715699    0.164770    Biso  1.000000  N
  N8          1.0    0.917736    0.215646    0.164808    Biso  1.000000  N
  N9          1.0    0.980547    0.715662    0.164881    Biso  1.000000  N
  N10         1.0    0.294467    0.215750    0.165201    Biso  1.000000  N
  B1          1.0    0.085005    0.215727    0.164764    Biso  1.000000  B
  B2          1.0    0.147806    0.715883    0.164758    Biso  1.000000  B
  B3          1.0    0.210590    0.215932    0.164905    Biso  1.000000  B
  B4          1.0    0.707998    0.215654    0.165251    Biso  1.000000  B
  B5          1.0    0.770957    0.715731    0.165072    Biso  1.000000  B

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B6	1.0	0.833773	0.215707	0.164828	Biso	1.000000	B
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B9	1.0	0.022190	0.715640	0.164811	Biso	1.000000	B
B10	1.0	0.273334	0.715774	0.165107	Biso	1.000000	B
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C5	1.0	0.478340	0.715470	0.165450	Biso	1.000000	C
C6	1.0	0.457975	0.215473	0.165476	Biso	1.000000	C
C7	1.0	0.539961	0.215517	0.165426	Biso	1.000000	C
C8	1.0	0.519579	0.715506	0.165423	Biso	1.000000	C
C9	1.0	0.601614	0.715402	0.165443	Biso	1.000000	C
C10	1.0	0.581256	0.215436	0.165442	Biso	1.000000	C
C11	1.0	0.663441	0.215482	0.165362	Biso	1.000000	C
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ZGNR(558)/hBN-7

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_cell_volume                   3584.147030
_space_group_name_H-M_alt      'P 1'
_space_group_IT_number         1

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B4	1.0	0.137960	0.352455	0.381950	Biso	1.000000	B
B5	1.0	0.258822	0.353147	0.383272	Biso	1.000000	B
B6	1.0	0.774998	0.352638	0.378305	Biso	1.000000	B
B7	1.0	0.714458	0.102835	0.378410	Biso	1.000000	B
B8	1.0	0.835508	0.102273	0.378932	Biso	1.000000	B
B9	1.0	0.896026	0.352147	0.380209	Biso	1.000000	B
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C25	1.0	0.318191	0.602853	0.384492	Biso	1.000000	C
C26	1.0	0.317906	0.102853	0.384469	Biso	1.000000	C

ZGNR(558)/hBN-5

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B4	1.0	0.160455	0.334088	0.380636	Biso	1.000000 B
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B6	1.0	0.748453	0.334286	0.382974	Biso	1.000000 B
B7	1.0	0.679762	0.082597	0.383739	Biso	1.000000 B
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B10	1.0	0.091837	0.084119	0.380732	Biso	1.000000 B
B11	1.0	0.954582	0.584181	0.383152	Biso	1.000000 B
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B16	1.0	0.679762	0.585680	0.383752	Biso	1.000000 B
B17	1.0	0.817269	0.584111	0.383251	Biso	1.000000 B
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N10	1.0	0.977720	0.834168	0.382841	Biso	1.000000 N
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N13	1.0	0.115010	0.834117	0.380471	Biso	1.000000 N
N14	1.0	0.252212	0.833971	0.382913	Biso	1.000000 N
N15	1.0	0.703209	0.834160	0.383239	Biso	1.000000 N
N16	1.0	0.840389	0.834264	0.383423	Biso	1.000000 N
N17	1.0	0.771749	0.584026	0.382949	Biso	1.000000 N
N18	1.0	0.909067	0.584255	0.383575	Biso	1.000000 N
N19	1.0	0.046357	0.584180	0.381475	Biso	1.000000 N

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C2	1.0	0.387848	0.833826	0.388214	Biso	1.000000	C
C3	1.0	0.630919	0.081108	0.385055	Biso	1.000000	C
C4	1.0	0.607625	0.834009	0.385844	Biso	1.000000	C
C5	1.0	0.364794	0.586277	0.387578	Biso	1.000000	C
C6	1.0	0.385692	0.333850	0.388328	Biso	1.000000	C
C7	1.0	0.630922	0.586980	0.385072	Biso	1.000000	C
C8	1.0	0.609900	0.334029	0.385838	Biso	1.000000	C
C9	1.0	0.454722	0.092852	0.389311	Biso	1.000000	C
C10	1.0	0.497565	0.189825	0.389222	Biso	1.000000	C
C11	1.0	0.497561	0.477961	0.389217	Biso	1.000000	C
C12	1.0	0.540719	0.093030	0.388061	Biso	1.000000	C
C13	1.0	0.565547	0.333971	0.387334	Biso	1.000000	C
C14	1.0	0.540713	0.574863	0.388062	Biso	1.000000	C
C15	1.0	0.560816	0.833955	0.387397	Biso	1.000000	C
C16	1.0	0.434541	0.833800	0.389078	Biso	1.000000	C
C17	1.0	0.429844	0.333808	0.389263	Biso	1.000000	C
C18	1.0	0.454719	0.574778	0.389310	Biso	1.000000	C

ZGNR(558)/hBN-9

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_cell_length_b                  4.968222
_cell_length_c                  20.000000
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_cell_angle_beta                90.000000
_cell_angle_gamma               90.000000
_cell_volume                    4006.030126
_space_group_name_H-M_alt       'P 1'
_space_group_IT_number          1

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loop_
_space_group_symop_operation_xyz
  'x, y, z'

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loop_
_atom_site_label
_atom_site_occupancy
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_adp_type

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<u>_atom_site_U_iso_or_equiv</u>					
<u>_atom_site_type_symbol</u>					
B1	1.0	0.071650	0.584453	0.381404	Biso 1.000000 B
B2	1.0	0.963489	0.084474	0.381670	Biso 1.000000 B
B3	1.0	0.179750	0.584427	0.383460	Biso 1.000000 B
B4	1.0	0.125711	0.334431	0.382006	Biso 1.000000 B
B5	1.0	0.233743	0.334406	0.385509	Biso 1.000000 B
B6	1.0	0.801214	0.334412	0.382078	Biso 1.000000 B
B7	1.0	0.746969	0.084603	0.382278	Biso 1.000000 B
B8	1.0	0.855310	0.084391	0.381983	Biso 1.000000 B
B9	1.0	0.909400	0.334429	0.381867	Biso 1.000000 B
B10	1.0	0.071650	0.084459	0.381404	Biso 1.000000 B
B11	1.0	0.963489	0.584473	0.381670	Biso 1.000000 B
B12	1.0	0.179750	0.084439	0.383461	Biso 1.000000 B
B13	1.0	0.125709	0.834433	0.382007	Biso 1.000000 B
B14	1.0	0.233767	0.834419	0.385514	Biso 1.000000 B
B15	1.0	0.801192	0.834404	0.382081	Biso 1.000000 B
B16	1.0	0.746966	0.584229	0.382277	Biso 1.000000 B
B17	1.0	0.855311	0.584423	0.381983	Biso 1.000000 B
B18	1.0	0.909401	0.834430	0.381867	Biso 1.000000 B
B19	1.0	0.017573	0.334473	0.381416	Biso 1.000000 B
B20	1.0	0.017573	0.834473	0.381416	Biso 1.000000 B
N1	1.0	0.981753	0.334491	0.381577	Biso 1.000000 N
N2	1.0	0.143999	0.584462	0.382345	Biso 1.000000 N
N3	1.0	0.251998	0.584243	0.386226	Biso 1.000000 N
N4	1.0	0.089925	0.334472	0.381489	Biso 1.000000 N
N5	1.0	0.198056	0.334437	0.384094	Biso 1.000000 N
N6	1.0	0.765327	0.334439	0.382168	Biso 1.000000 N
N7	1.0	0.873570	0.334427	0.381954	Biso 1.000000 N
N8	1.0	0.819473	0.084382	0.382046	Biso 1.000000 N
N9	1.0	0.927662	0.084454	0.381815	Biso 1.000000 N
N10	1.0	0.981753	0.834492	0.381578	Biso 1.000000 N
N11	1.0	0.144000	0.084439	0.382346	Biso 1.000000 N
N12	1.0	0.252002	0.084589	0.386229	Biso 1.000000 N
N13	1.0	0.089925	0.834472	0.381490	Biso 1.000000 N
N14	1.0	0.198081	0.834438	0.384098	Biso 1.000000 N
N15	1.0	0.765276	0.834426	0.382163	Biso 1.000000 N
N16	1.0	0.873572	0.834430	0.381954	Biso 1.000000 N
N17	1.0	0.819474	0.584465	0.382044	Biso 1.000000 N
N18	1.0	0.927661	0.584458	0.381814	Biso 1.000000 N
N19	1.0	0.035843	0.584486	0.381357	Biso 1.000000 N
N20	1.0	0.035843	0.084488	0.381357	Biso 1.000000 N
C1	1.0	0.392697	0.081649	0.389360	Biso 1.000000 C
C2	1.0	0.411159	0.834373	0.389323	Biso 1.000000 C

C3	1.0	0.602227	0.081852	0.385118	Biso	1.000000	C
C4	1.0	0.637766	0.083136	0.384134	Biso	1.000000	C
C5	1.0	0.583746	0.834413	0.385669	Biso	1.000000	C
C6	1.0	0.655464	0.834480	0.383674	Biso	1.000000	C
C7	1.0	0.392702	0.587035	0.389352	Biso	1.000000	C
C8	1.0	0.409441	0.334313	0.389423	Biso	1.000000	C
C9	1.0	0.602227	0.587005	0.385087	Biso	1.000000	C
C10	1.0	0.637773	0.585829	0.384117	Biso	1.000000	C
C11	1.0	0.585499	0.334418	0.385613	Biso	1.000000	C
C12	1.0	0.655206	0.334466	0.383703	Biso	1.000000	C
C13	1.0	0.463736	0.093146	0.388893	Biso	1.000000	C
C14	1.0	0.497450	0.189293	0.388272	Biso	1.000000	C
C15	1.0	0.497444	0.479632	0.388272	Biso	1.000000	C
C16	1.0	0.531210	0.093338	0.387318	Biso	1.000000	C
C17	1.0	0.550857	0.334542	0.386725	Biso	1.000000	C
C18	1.0	0.531206	0.575831	0.387310	Biso	1.000000	C
C19	1.0	0.547314	0.834524	0.386809	Biso	1.000000	C
C20	1.0	0.447647	0.834373	0.389075	Biso	1.000000	C
C21	1.0	0.444041	0.334354	0.389218	Biso	1.000000	C
C22	1.0	0.463731	0.575645	0.388901	Biso	1.000000	C
C23	1.0	0.357180	0.585711	0.389031	Biso	1.000000	C
C24	1.0	0.357175	0.082981	0.389041	Biso	1.000000	C
C25	1.0	0.339778	0.334351	0.388752	Biso	1.000000	C
C26	1.0	0.339550	0.834345	0.388748	Biso	1.000000	C
C27	1.0	0.304082	0.334374	0.387917	Biso	1.000000	C
C28	1.0	0.286716	0.584185	0.387396	Biso	1.000000	C
C29	1.0	0.286717	0.084554	0.387401	Biso	1.000000	C
C30	1.0	0.303897	0.834366	0.387914	Biso	1.000000	C
C31	1.0	0.691002	0.334497	0.382948	Biso	1.000000	C
C32	1.0	0.708587	0.584197	0.382643	Biso	1.000000	C
C33	1.0	0.708589	0.084792	0.382650	Biso	1.000000	C
C34	1.0	0.691203	0.834499	0.382932	Biso	1.000000	C

ZGNR(558)/hBN-11

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_cell_length_a	44.593498	
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_cell_angle_gamma	90.000000	
_cell_volume	4427.872965	
_space_group_name_H-M_alt	' P 1'	

\_space\_group\_IT\_number

1

loop\_

\_space\_group\_symop\_operation\_xyz

'x, y, z'

loop\_

\_atom\_site\_label

\_atom\_site\_occupancy

\_atom\_site\_fract\_x

\_atom\_site\_fract\_y

\_atom\_site\_fract\_z

\_atom\_site\_adp\_type

\_atom\_site\_U\_iso\_or\_equiv

\_atom\_site\_type\_symbol

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B2	1.0	0.010595	0.628766	0.381518	Biso	1.000000	B
B3	1.0	0.108365	0.628798	0.381379	Biso	1.000000	B
B4	1.0	0.912807	0.128801	0.381672	Biso	1.000000	B
B5	1.0	0.206084	0.628922	0.383558	Biso	1.000000	B
B6	1.0	0.157230	0.378854	0.382001	Biso	1.000000	B
B7	1.0	0.765967	0.378863	0.381964	Biso	1.000000	B
B8	1.0	0.814995	0.128861	0.381882	Biso	1.000000	B
B9	1.0	0.863900	0.378811	0.381780	Biso	1.000000	B
B10	1.0	0.108365	0.128807	0.381378	Biso	1.000000	B
B11	1.0	0.912807	0.628799	0.381672	Biso	1.000000	B
B12	1.0	0.206084	0.128938	0.383558	Biso	1.000000	B
B13	1.0	0.157227	0.878855	0.382001	Biso	1.000000	B
B14	1.0	0.765964	0.878867	0.381962	Biso	1.000000	B
B15	1.0	0.814995	0.628884	0.381882	Biso	1.000000	B
B16	1.0	0.863902	0.878811	0.381780	Biso	1.000000	B
B17	1.0	0.059477	0.378742	0.381372	Biso	1.000000	B
B18	1.0	0.059477	0.878742	0.381372	Biso	1.000000	B
B19	1.0	0.961695	0.378777	0.381582	Biso	1.000000	B
B20	1.0	0.961695	0.878777	0.381584	Biso	1.000000	B
N1	1.0	0.027106	0.378758	0.381490	Biso	1.000000	N
N2	1.0	0.027106	0.878758	0.381490	Biso	1.000000	N
N3	1.0	0.929311	0.378797	0.381639	Biso	1.000000	N
N4	1.0	0.173797	0.628885	0.382376	Biso	1.000000	N
N5	1.0	0.124898	0.378806	0.381462	Biso	1.000000	N
N6	1.0	0.222564	0.378968	0.384245	Biso	1.000000	N
N7	1.0	0.831503	0.378857	0.381861	Biso	1.000000	N
N8	1.0	0.782534	0.128832	0.381932	Biso	1.000000	N
N9	1.0	0.880411	0.128808	0.381750	Biso	1.000000	N

N10	1.0	0.929311	0.878797	0.381642	Biso	1.000000 N
N11	1.0	0.173797	0.128862	0.382376	Biso	1.000000 N
N12	1.0	0.124898	0.878806	0.381463	Biso	1.000000 N
N13	1.0	0.222591	0.878967	0.384248	Biso	1.000000 N
N14	1.0	0.831505	0.878857	0.381860	Biso	1.000000 N
N15	1.0	0.782534	0.628893	0.381931	Biso	1.000000 N
N16	1.0	0.880411	0.628805	0.381750	Biso	1.000000 N
N17	1.0	0.076001	0.628742	0.381333	Biso	1.000000 N
N18	1.0	0.076001	0.128745	0.381333	Biso	1.000000 N
N19	1.0	0.978209	0.628773	0.381572	Biso	1.000000 N
N20	1.0	0.978209	0.128772	0.381572	Biso	1.000000 N
C1	1.0	0.253971	0.379119	0.385592	Biso	1.000000 C
C2	1.0	0.715464	0.129092	0.382262	Biso	1.000000 C
C3	1.0	0.254006	0.879119	0.385593	Biso	1.000000 C
C4	1.0	0.715466	0.628735	0.382260	Biso	1.000000 C
C5	1.0	0.269601	0.629003	0.386244	Biso	1.000000 C
C6	1.0	0.731295	0.378894	0.382122	Biso	1.000000 C
C7	1.0	0.269601	0.129292	0.386243	Biso	1.000000 C
C8	1.0	0.731252	0.878900	0.382118	Biso	1.000000 C
C9	1.0	0.397741	0.126540	0.389253	Biso	1.000000 C
C10	1.0	0.414474	0.879223	0.389233	Biso	1.000000 C
C11	1.0	0.587196	0.126559	0.385163	Biso	1.000000 C
C12	1.0	0.619233	0.127668	0.384142	Biso	1.000000 C
C13	1.0	0.570458	0.879188	0.385761	Biso	1.000000 C
C14	1.0	0.635266	0.878981	0.383692	Biso	1.000000 C
C15	1.0	0.397742	0.631920	0.389245	Biso	1.000000 C
C16	1.0	0.412914	0.379208	0.389322	Biso	1.000000 C
C17	1.0	0.587194	0.631754	0.385180	Biso	1.000000 C
C18	1.0	0.619230	0.630384	0.384147	Biso	1.000000 C
C19	1.0	0.572035	0.379176	0.385710	Biso	1.000000 C
C20	1.0	0.635041	0.378991	0.383710	Biso	1.000000 C
C21	1.0	0.461993	0.137846	0.388919	Biso	1.000000 C
C22	1.0	0.492477	0.233783	0.388365	Biso	1.000000 C
C23	1.0	0.492473	0.524604	0.388360	Biso	1.000000 C
C24	1.0	0.522975	0.137905	0.387408	Biso	1.000000 C
C25	1.0	0.540755	0.379233	0.386825	Biso	1.000000 C
C26	1.0	0.522970	0.620508	0.387416	Biso	1.000000 C
C27	1.0	0.537579	0.879189	0.386898	Biso	1.000000 C
C28	1.0	0.447397	0.879179	0.389062	Biso	1.000000 C
C29	1.0	0.444182	0.379168	0.389191	Biso	1.000000 C
C30	1.0	0.461990	0.620458	0.388916	Biso	1.000000 C
C31	1.0	0.365695	0.630626	0.388967	Biso	1.000000 C
C32	1.0	0.365697	0.127847	0.388978	Biso	1.000000 C
C33	1.0	0.349888	0.379231	0.388724	Biso	1.000000 C

C34	1.0	0.349674	0.879239	0.388713	Biso	1.000000	C
C35	1.0	0.317771	0.379250	0.387942	Biso	1.000000	C
C36	1.0	0.301850	0.629044	0.387445	Biso	1.000000	C
C37	1.0	0.301850	0.129424	0.387447	Biso	1.000000	C
C38	1.0	0.317588	0.879242	0.387926	Biso	1.000000	C
C39	1.0	0.667170	0.378948	0.382970	Biso	1.000000	C
C40	1.0	0.683142	0.628707	0.382672	Biso	1.000000	C
C41	1.0	0.683140	0.129161	0.382677	Biso	1.000000	C
C42	1.0	0.667343	0.878939	0.382953	Biso	1.000000	C

ZGNR(558)/hBN-13

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_cell_volume	4849.770711						
_space_group_name_H-M_alt	'P 1'						
_space_group_IT_number	1						

loop\_  
 \_space\_group\_symop\_operation\_xyz  
 'x, y, z'

loop_ _atom_site_label							
_atom_site_occupancy							
_atom_site_fract_x							
_atom_site_fract_y							
_atom_site_fract_z							
_atom_site_adp_type							
_atom_site_U_iso_or_equiv							
_atom_site_type_symbol							
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B2	1.0	0.011035	0.855114	0.395030	Biso	1.000000	B
B3	1.0	0.055663	0.105216	0.395004	Biso	1.000000	B
B4	1.0	0.055663	0.605215	0.395005	Biso	1.000000	B
B5	1.0	0.144891	0.605269	0.394935	Biso	1.000000	B
B6	1.0	0.877117	0.105292	0.395229	Biso	1.000000	B
B7	1.0	0.189476	0.355182	0.395797	Biso	1.000000	B
B8	1.0	0.787699	0.105319	0.395241	Biso	1.000000	B

B9	1.0	0.832460	0.355251	0.395280	Biso	1.000000	B
B10	1.0	0.144891	0.105284	0.394935	Biso	1.000000	B
B11	1.0	0.877117	0.605292	0.395230	Biso	1.000000	B
B12	1.0	0.189475	0.855182	0.395796	Biso	1.000000	B
B13	1.0	0.787699	0.605327	0.395241	Biso	1.000000	B
B14	1.0	0.832462	0.855251	0.395280	Biso	1.000000	B
B15	1.0	0.100286	0.355109	0.394744	Biso	1.000000	B
B16	1.0	0.100286	0.855108	0.394744	Biso	1.000000	B
B17	1.0	0.921762	0.355155	0.395008	Biso	1.000000	B
B18	1.0	0.921763	0.855155	0.395008	Biso	1.000000	B
B19	1.0	0.966399	0.105252	0.394918	Biso	1.000000	B
B20	1.0	0.966399	0.605252	0.394918	Biso	1.000000	B
N1	1.0	0.026110	0.605117	0.395076	Biso	1.000000	N
N2	1.0	0.026110	0.105117	0.395075	Biso	1.000000	N
N3	1.0	0.070745	0.355188	0.394924	Biso	1.000000	N
N4	1.0	0.070745	0.855188	0.394924	Biso	1.000000	N
N5	1.0	0.892189	0.355260	0.395184	Biso	1.000000	N
N6	1.0	0.204525	0.605169	0.396232	Biso	1.000000	N
N7	1.0	0.160005	0.355255	0.395112	Biso	1.000000	N
N8	1.0	0.802829	0.355311	0.395274	Biso	1.000000	N
N9	1.0	0.847538	0.105256	0.395275	Biso	1.000000	N
N10	1.0	0.892189	0.855260	0.395184	Biso	1.000000	N
N11	1.0	0.204526	0.105169	0.396232	Biso	1.000000	N
N12	1.0	0.160006	0.855256	0.395111	Biso	1.000000	N
N13	1.0	0.802828	0.855311	0.395275	Biso	1.000000	N
N14	1.0	0.847538	0.605258	0.395276	Biso	1.000000	N
N15	1.0	0.115377	0.605130	0.394688	Biso	1.000000	N
N16	1.0	0.115377	0.105131	0.394688	Biso	1.000000	N
N17	1.0	0.936832	0.605162	0.394924	Biso	1.000000	N
N18	1.0	0.936832	0.105163	0.394924	Biso	1.000000	N
N19	1.0	0.981472	0.355223	0.394928	Biso	1.000000	N
N20	1.0	0.981472	0.855223	0.394928	Biso	1.000000	N
C1	1.0	0.233201	0.605118	0.397312	Biso	1.000000	C
C2	1.0	0.276845	0.355101	0.398983	Biso	1.000000	C
C3	1.0	0.741601	0.355044	0.395239	Biso	1.000000	C
C4	1.0	0.697615	0.105193	0.395707	Biso	1.000000	C
C5	1.0	0.233201	0.105093	0.397312	Biso	1.000000	C
C6	1.0	0.276877	0.855100	0.398970	Biso	1.000000	C
C7	1.0	0.741593	0.855046	0.395239	Biso	1.000000	C
C8	1.0	0.697616	0.604881	0.395696	Biso	1.000000	C
C9	1.0	0.291300	0.604953	0.399482	Biso	1.000000	C
C10	1.0	0.247442	0.355092	0.397875	Biso	1.000000	C
C11	1.0	0.712132	0.355019	0.395492	Biso	1.000000	C
C12	1.0	0.756031	0.105068	0.395189	Biso	1.000000	C

C13	1.0	0.291300	0.105221	0.399478	Biso	1.000000	C
C14	1.0	0.247450	0.855090	0.397863	Biso	1.000000	C
C15	1.0	0.712101	0.855025	0.395494	Biso	1.000000	C
C16	1.0	0.756031	0.605094	0.395188	Biso	1.000000	C
C17	1.0	0.408018	0.102505	0.402204	Biso	1.000000	C
C18	1.0	0.423308	0.855197	0.402188	Biso	1.000000	C
C19	1.0	0.580864	0.102282	0.398670	Biso	1.000000	C
C20	1.0	0.610054	0.103569	0.397796	Biso	1.000000	C
C21	1.0	0.565566	0.854955	0.399121	Biso	1.000000	C
C22	1.0	0.624708	0.854982	0.397354	Biso	1.000000	C
C23	1.0	0.408016	0.607882	0.402193	Biso	1.000000	C
C24	1.0	0.421865	0.355185	0.402230	Biso	1.000000	C
C25	1.0	0.580865	0.607593	0.398627	Biso	1.000000	C
C26	1.0	0.610052	0.606369	0.397767	Biso	1.000000	C
C27	1.0	0.567021	0.354958	0.399129	Biso	1.000000	C
C28	1.0	0.624503	0.354985	0.397373	Biso	1.000000	C
C29	1.0	0.466636	0.113857	0.401827	Biso	1.000000	C
C30	1.0	0.494439	0.209523	0.401331	Biso	1.000000	C
C31	1.0	0.494442	0.500722	0.401341	Biso	1.000000	C
C32	1.0	0.522248	0.113714	0.400559	Biso	1.000000	C
C33	1.0	0.538496	0.355034	0.400076	Biso	1.000000	C
C34	1.0	0.522252	0.596423	0.400557	Biso	1.000000	C
C35	1.0	0.535597	0.855068	0.400107	Biso	1.000000	C
C36	1.0	0.453299	0.855205	0.401978	Biso	1.000000	C
C37	1.0	0.450384	0.355226	0.402080	Biso	1.000000	C
C38	1.0	0.466639	0.596557	0.401833	Biso	1.000000	C
C39	1.0	0.378824	0.606629	0.401937	Biso	1.000000	C
C40	1.0	0.378826	0.103789	0.401936	Biso	1.000000	C
C41	1.0	0.364380	0.355223	0.401691	Biso	1.000000	C
C42	1.0	0.364180	0.855211	0.401671	Biso	1.000000	C
C43	1.0	0.335159	0.355198	0.400928	Biso	1.000000	C
C44	1.0	0.320567	0.604989	0.400462	Biso	1.000000	C
C45	1.0	0.320567	0.105374	0.400464	Biso	1.000000	C
C46	1.0	0.334996	0.855201	0.400906	Biso	1.000000	C
C47	1.0	0.653729	0.355079	0.396599	Biso	1.000000	C
C48	1.0	0.668338	0.604854	0.396245	Biso	1.000000	C
C49	1.0	0.668337	0.105261	0.396259	Biso	1.000000	C
C50	1.0	0.653885	0.855066	0.396580	Biso	1.000000	C

ZGNR(558)/hBN-7(04)

\_chemical\_name\_common  
\_cell\_length\_a  
\_cell\_length\_b

' POSCAR-704  
36.005692  
4.976215

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  _atom_site_fract_z
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  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
  B1      1.0    0.957493    0.574685    0.382312    Biso  1.000000 B
  B2      1.0    0.836388    0.074855    0.381500    Biso  1.000000 B
  B3      1.0    0.078567    0.575089    0.382224    Biso  1.000000 B
  B4      1.0    0.018046    0.324874    0.381970    Biso  1.000000 B
  B5      1.0    0.139109    0.325227    0.383236    Biso  1.000000 B
  B6      1.0    0.715105    0.075039    0.378963    Biso  1.000000 B
  B7      1.0    0.775820    0.324869    0.380180    Biso  1.000000 B
  B8      1.0    0.957490    0.074686    0.382312    Biso  1.000000 B
  B9      1.0    0.836385    0.574855    0.381500    Biso  1.000000 B
  B10     1.0    0.078601    0.075080    0.382225    Biso  1.000000 B
  B11     1.0    0.018046    0.824925    0.381970    Biso  1.000000 B
  B12     1.0    0.139111    0.824696    0.383240    Biso  1.000000 B
  B13     1.0    0.715112    0.575039    0.378961    Biso  1.000000 B
  B14     1.0    0.775820    0.824887    0.380180    Biso  1.000000 B
  B15     1.0    0.896933    0.324665    0.382268    Biso  1.000000 B
  B16     1.0    0.896933    0.824658    0.382268    Biso  1.000000 B
  B17     1.0    0.260096    0.321261    0.385113    Biso  1.000000 B
  B18     1.0    0.260102    0.828531    0.385114    Biso  1.000000 B
  B19     1.0    0.199805    0.574949    0.384507    Biso  1.000000 B
  B20     1.0    0.199438    0.074950    0.384508    Biso  1.000000 B
  C1      1.0    0.652546    0.325113    0.378404    Biso  1.000000 C
  C2      1.0    0.592972    0.074922    0.378499    Biso  1.000000 C
  C3      1.0    0.652547    0.824821    0.378400    Biso  1.000000 C

```

C4	1.0	0.592743	0.574931	0.378490	Biso	1.000000	C
C5	1.0	0.612499	0.325111	0.378393	Biso	1.000000	C
C6	1.0	0.672071	0.074972	0.378498	Biso	1.000000	C
C7	1.0	0.612500	0.824780	0.378392	Biso	1.000000	C
C8	1.0	0.672118	0.574962	0.378496	Biso	1.000000	C
C9	1.0	0.493718	0.321994	0.379943	Biso	1.000000	C
C10	1.0	0.533396	0.323449	0.379190	Biso	1.000000	C
C11	1.0	0.473031	0.074924	0.380448	Biso	1.000000	C
C12	1.0	0.553225	0.074962	0.378924	Biso	1.000000	C
C13	1.0	0.493715	0.827870	0.379948	Biso	1.000000	C
C14	1.0	0.533395	0.826513	0.379192	Biso	1.000000	C
C15	1.0	0.474981	0.574911	0.380361	Biso	1.000000	C
C16	1.0	0.552939	0.574983	0.378882	Biso	1.000000	C
C17	1.0	0.338916	0.333282	0.384096	Biso	1.000000	C
C18	1.0	0.376755	0.429515	0.383136	Biso	1.000000	C
C19	1.0	0.376748	0.720410	0.383143	Biso	1.000000	C
C20	1.0	0.414356	0.333279	0.382005	Biso	1.000000	C
C21	1.0	0.436337	0.574939	0.381380	Biso	1.000000	C
C22	1.0	0.414353	0.816640	0.382039	Biso	1.000000	C
C23	1.0	0.432272	0.074937	0.381523	Biso	1.000000	C
C24	1.0	0.321490	0.074979	0.384386	Biso	1.000000	C
C25	1.0	0.317250	0.574936	0.384560	Biso	1.000000	C
C26	1.0	0.338907	0.816642	0.384076	Biso	1.000000	C
N1	1.0	0.856762	0.324828	0.381879	Biso	1.000000	N
N2	1.0	0.038421	0.574926	0.381921	Biso	1.000000	N
N3	1.0	0.159635	0.574959	0.383679	Biso	1.000000	N
N4	1.0	0.977878	0.324720	0.382192	Biso	1.000000	N
N5	1.0	0.098979	0.325198	0.382457	Biso	1.000000	N
N6	1.0	0.735567	0.324977	0.379286	Biso	1.000000	N
N7	1.0	0.796205	0.074868	0.380665	Biso	1.000000	N
N8	1.0	0.856762	0.824821	0.381879	Biso	1.000000	N
N9	1.0	0.038441	0.074922	0.381922	Biso	1.000000	N
N10	1.0	0.159415	0.074964	0.383673	Biso	1.000000	N
N11	1.0	0.977878	0.824746	0.382192	Biso	1.000000	N
N12	1.0	0.098981	0.824925	0.382459	Biso	1.000000	N
N13	1.0	0.735567	0.825038	0.379285	Biso	1.000000	N
N14	1.0	0.796202	0.574867	0.380665	Biso	1.000000	N
N15	1.0	0.917318	0.574672	0.382401	Biso	1.000000	N
N16	1.0	0.917316	0.074672	0.382401	Biso	1.000000	N
N17	1.0	0.281677	0.074930	0.384970	Biso	1.000000	N
N18	1.0	0.279332	0.574907	0.385148	Biso	1.000000	N
N19	1.0	0.220074	0.826462	0.384899	Biso	1.000000	N
N20	1.0	0.220071	0.323450	0.384900	Biso	1.000000	N

ZGNR(558)/hBN-7(13)

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_chemical_name_common          'POSCAR-713'  
_cell_length_a                 36.029007  
_cell_length_b                 4.973705  
_cell_length_c                 20.000000  
_cell_angle_alpha              90.000000  
_cell_angle_beta               90.000000  
_cell_angle_gamma              90.000000  
_cell_volume                    3583.952908  
_space_group_name_H-M_alt      'P 1'  
_space_group_IT_number         1
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loop_  
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  'x, y, z'
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  _atom_site_fract_x  
  _atom_site_fract_y  
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  _atom_site_adp_type  
  _atom_site_U_iso_or_equiv  
  _atom_site_type_symbol  
B1      1.0    0.022472    0.592036    0.382224    Biso  1.000000 B  
B2      1.0    0.901450    0.091976    0.381606    Biso  1.000000 B  
B3      1.0    0.143445    0.592383    0.382194    Biso  1.000000 B  
B4      1.0    0.082966    0.342282    0.381948    Biso  1.000000 B  
B5      1.0    0.203931    0.342671    0.383255    Biso  1.000000 B  
B6      1.0    0.719761    0.342754    0.378271    Biso  1.000000 B  
B7      1.0    0.780419    0.092280    0.378929    Biso  1.000000 B  
B8      1.0    0.840948    0.342233    0.380247    Biso  1.000000 B  
B9      1.0    0.022469    0.092036    0.382224    Biso  1.000000 B  
B10     1.0    0.901448    0.591977    0.381606    Biso  1.000000 B  
B11     1.0    0.143472    0.092381    0.382192    Biso  1.000000 B  
B12     1.0    0.082966    0.842316    0.381949    Biso  1.000000 B  
B13     1.0    0.203930    0.842143    0.383257    Biso  1.000000 B  
B14     1.0    0.719760    0.842429    0.378269    Biso  1.000000 B  
B15     1.0    0.780437    0.592285    0.378927    Biso  1.000000 B  
B16     1.0    0.840949    0.842258    0.380246    Biso  1.000000 B  
B17     1.0    0.961964    0.341907    0.382300    Biso  1.000000 B  
B18     1.0    0.961964    0.841898    0.382301    Biso  1.000000 B  
B19     1.0    0.264505    0.592541    0.384571    Biso  1.000000 B
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B20	1.0	0.264209	0.092534	0.384561	Biso	1.000000	B
C1	1.0	0.657363	0.092748	0.378452	Biso	1.000000	C
C2	1.0	0.657140	0.592744	0.378453	Biso	1.000000	C
C3	1.0	0.676797	0.342957	0.378315	Biso	1.000000	C
C4	1.0	0.676796	0.842443	0.378317	Biso	1.000000	C
C5	1.0	0.323600	0.340394	0.385062	Biso	1.000000	C
C6	1.0	0.343912	0.092847	0.384956	Biso	1.000000	C
C7	1.0	0.557798	0.340235	0.379965	Biso	1.000000	C
C8	1.0	0.597580	0.341468	0.379185	Biso	1.000000	C
C9	1.0	0.537149	0.092952	0.380478	Biso	1.000000	C
C10	1.0	0.617359	0.092871	0.378876	Biso	1.000000	C
C11	1.0	0.323607	0.845188	0.385045	Biso	1.000000	C
C12	1.0	0.342018	0.592806	0.385044	Biso	1.000000	C
C13	1.0	0.557799	0.845616	0.379979	Biso	1.000000	C
C14	1.0	0.597583	0.844286	0.379187	Biso	1.000000	C
C15	1.0	0.539102	0.592963	0.380411	Biso	1.000000	C
C16	1.0	0.617072	0.592870	0.378888	Biso	1.000000	C
C17	1.0	0.402867	0.351656	0.384107	Biso	1.000000	C
C18	1.0	0.440651	0.447852	0.383195	Biso	1.000000	C
C19	1.0	0.440647	0.738028	0.383195	Biso	1.000000	C
C20	1.0	0.478393	0.351651	0.382092	Biso	1.000000	C
C21	1.0	0.500370	0.592989	0.381444	Biso	1.000000	C
C22	1.0	0.478390	0.834316	0.382092	Biso	1.000000	C
C23	1.0	0.496354	0.092985	0.381579	Biso	1.000000	C
C24	1.0	0.385013	0.092889	0.384451	Biso	1.000000	C
C25	1.0	0.380979	0.592846	0.384602	Biso	1.000000	C
C26	1.0	0.402858	0.834125	0.384127	Biso	1.000000	C
N1	1.0	0.921853	0.341970	0.381983	Biso	1.000000	N
N2	1.0	0.103379	0.592307	0.381907	Biso	1.000000	N
N3	1.0	0.224489	0.592444	0.383740	Biso	1.000000	N
N4	1.0	0.042879	0.342070	0.382113	Biso	1.000000	N
N5	1.0	0.163900	0.342498	0.382414	Biso	1.000000	N
N6	1.0	0.800833	0.342238	0.379292	Biso	1.000000	N
N7	1.0	0.740218	0.092525	0.378359	Biso	1.000000	N
N8	1.0	0.861346	0.092188	0.380763	Biso	1.000000	N
N9	1.0	0.921853	0.841963	0.381985	Biso	1.000000	N
N10	1.0	0.103396	0.092307	0.381906	Biso	1.000000	N
N11	1.0	0.224322	0.092439	0.383732	Biso	1.000000	N
N12	1.0	0.042879	0.842092	0.382113	Biso	1.000000	N
N13	1.0	0.163899	0.842273	0.382415	Biso	1.000000	N
N14	1.0	0.800833	0.842300	0.379291	Biso	1.000000	N
N15	1.0	0.740265	0.592532	0.378356	Biso	1.000000	N
N16	1.0	0.861342	0.592190	0.380762	Biso	1.000000	N
N17	1.0	0.982369	0.591937	0.382368	Biso	1.000000	N

N18	1.0	0.982368	0.091937	0.382367	Biso	1.000000	N
N19	1.0	0.284780	0.843962	0.384891	Biso	1.000000	N
N20	1.0	0.284777	0.341252	0.384901	Biso	1.000000	N

ZGNR(558)/hBN-7(31)

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_space_group_IT_number	1

loop\_

_space_group_symop_operation_xyz	'x, y, z'
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loop\_

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_atom_site_fract_x							
_atom_site_fract_y							
_atom_site_fract_z							
_atom_site_adp_type							
_atom_site_U_iso_or_equiv							
_atom_site_type_symbol							
B1	1.0	0.141613	0.607595	0.382289	Biso	1.000000	B
B2	1.0	0.020670	0.107769	0.381475	Biso	1.000000	B
B3	1.0	0.262441	0.607404	0.382532	Biso	1.000000	B
B4	1.0	0.202047	0.357418	0.382134	Biso	1.000000	B
B5	1.0	0.839212	0.357563	0.378349	Biso	1.000000	B
B6	1.0	0.778826	0.107522	0.378378	Biso	1.000000	B
B7	1.0	0.899701	0.107528	0.378989	Biso	1.000000	B
B8	1.0	0.960197	0.357533	0.380189	Biso	1.000000	B
B9	1.0	0.141609	0.107595	0.382289	Biso	1.000000	B
B10	1.0	0.020668	0.607770	0.381474	Biso	1.000000	B
B11	1.0	0.262468	0.107410	0.382529	Biso	1.000000	B
B12	1.0	0.202047	0.857376	0.382134	Biso	1.000000	B
B13	1.0	0.839212	0.857261	0.378350	Biso	1.000000	B
B14	1.0	0.778558	0.607508	0.378378	Biso	1.000000	B

B15	1.0	0.899722	0.607523	0.378990	Biso	1.000000	B
B16	1.0	0.960196	0.857560	0.380189	Biso	1.000000	B
B17	1.0	0.081145	0.357804	0.382268	Biso	1.000000	B
B18	1.0	0.081145	0.857795	0.382268	Biso	1.000000	B
B19	1.0	0.718016	0.355752	0.379040	Biso	1.000000	B
B20	1.0	0.718024	0.858820	0.379035	Biso	1.000000	B
C1	1.0	0.321710	0.357668	0.383410	Biso	1.000000	C
C2	1.0	0.321707	0.857307	0.383411	Biso	1.000000	C
C3	1.0	0.341150	0.607491	0.383751	Biso	1.000000	C
C4	1.0	0.340918	0.107490	0.383744	Biso	1.000000	C
C5	1.0	0.440299	0.354623	0.384743	Biso	1.000000	C
C6	1.0	0.460919	0.107444	0.384687	Biso	1.000000	C
C7	1.0	0.675015	0.354271	0.379933	Biso	1.000000	C
C8	1.0	0.654461	0.107137	0.380497	Biso	1.000000	C
C9	1.0	0.440299	0.860380	0.384757	Biso	1.000000	C
C10	1.0	0.459055	0.607443	0.384736	Biso	1.000000	C
C11	1.0	0.675020	0.860077	0.379928	Biso	1.000000	C
C12	1.0	0.656464	0.607152	0.380427	Biso	1.000000	C
C13	1.0	0.519758	0.366096	0.384109	Biso	1.000000	C
C14	1.0	0.557450	0.462499	0.383360	Biso	1.000000	C
C15	1.0	0.557450	0.751831	0.383356	Biso	1.000000	C
C16	1.0	0.595459	0.366129	0.382234	Biso	1.000000	C
C17	1.0	0.617365	0.607091	0.381581	Biso	1.000000	C
C18	1.0	0.595457	0.848107	0.382240	Biso	1.000000	C
C19	1.0	0.613242	0.107115	0.381687	Biso	1.000000	C
C20	1.0	0.501846	0.107272	0.384323	Biso	1.000000	C
C21	1.0	0.497705	0.607321	0.384461	Biso	1.000000	C
C22	1.0	0.519758	0.848433	0.384093	Biso	1.000000	C
C23	1.0	0.400545	0.858929	0.384581	Biso	1.000000	C
C24	1.0	0.400544	0.356119	0.384571	Biso	1.000000	C
C25	1.0	0.381066	0.607530	0.384368	Biso	1.000000	C
C26	1.0	0.380829	0.107534	0.384360	Biso	1.000000	C
N1	1.0	0.041102	0.357771	0.381860	Biso	1.000000	N
N2	1.0	0.222523	0.607404	0.382159	Biso	1.000000	N
N3	1.0	0.162066	0.357550	0.382202	Biso	1.000000	N
N4	1.0	0.282875	0.357628	0.382783	Biso	1.000000	N
N5	1.0	0.799135	0.357761	0.378268	Biso	1.000000	N
N6	1.0	0.920138	0.357502	0.379323	Biso	1.000000	N
N7	1.0	0.859625	0.107438	0.378450	Biso	1.000000	N
N8	1.0	0.980623	0.107591	0.380660	Biso	1.000000	N
N9	1.0	0.041102	0.857767	0.381860	Biso	1.000000	N
N10	1.0	0.222559	0.107406	0.382156	Biso	1.000000	N
N11	1.0	0.162067	0.857578	0.382202	Biso	1.000000	N
N12	1.0	0.282873	0.857232	0.382789	Biso	1.000000	N

N13	1.0	0.799134	0.857240	0.378268	Biso	1.000000	N
N14	1.0	0.920138	0.857554	0.379324	Biso	1.000000	N
N15	1.0	0.859660	0.607438	0.378452	Biso	1.000000	N
N16	1.0	0.980621	0.607592	0.380658	Biso	1.000000	N
N17	1.0	0.101588	0.607755	0.382388	Biso	1.000000	N
N18	1.0	0.101587	0.107755	0.382387	Biso	1.000000	N
N19	1.0	0.738724	0.107344	0.378705	Biso	1.000000	N
N20	1.0	0.738379	0.607328	0.378712	Biso	1.000000	N

ZGNR(558)/hBN-7(40)

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_cell_length_a	36.030510						
_cell_length_b	4.974988						
_cell_length_c	20.000000						
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_cell_volume	3585.027424						
_space_group_name_H-M_alt	'P 1'						
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loop\_

_space_group_symop_operation_xyz	'x, y, z'						
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loop\_

_atom_site_label							
_atom_site_occupancy							
_atom_site_fract_x							
_atom_site_fract_y							
_atom_site_fract_z							
_atom_site_adp_type							
_atom_site_U_iso_or_equiv							
_atom_site_type_symbol							
B1	1.0	0.200701	0.589453	0.382049	Biso	1.000000	B
B2	1.0	0.079776	0.089192	0.381475	Biso	1.000000	B
B3	1.0	0.261129	0.339311	0.382207	Biso	1.000000	B
B4	1.0	0.898329	0.338980	0.378396	Biso	1.000000	B
B5	1.0	0.837938	0.088843	0.378374	Biso	1.000000	B
B6	1.0	0.958808	0.088730	0.379146	Biso	1.000000	B
B7	1.0	0.019298	0.338977	0.380398	Biso	1.000000	B
B8	1.0	0.200697	0.089454	0.382049	Biso	1.000000	B
B9	1.0	0.079774	0.589191	0.381474	Biso	1.000000	B

B10	1.0	0.261129	0.839179	0.382209	Biso	1.000000	B
B11	1.0	0.898330	0.838735	0.378401	Biso	1.000000	B
B12	1.0	0.837725	0.588857	0.378391	Biso	1.000000	B
B13	1.0	0.958821	0.588727	0.379148	Biso	1.000000	B
B14	1.0	0.019298	0.838998	0.380398	Biso	1.000000	B
B15	1.0	0.140239	0.339487	0.381982	Biso	1.000000	B
B16	1.0	0.140239	0.839470	0.381981	Biso	1.000000	B
B17	1.0	0.777311	0.337534	0.379084	Biso	1.000000	B
B18	1.0	0.715692	0.088662	0.380523	Biso	1.000000	B
B19	1.0	0.777309	0.840250	0.379081	Biso	1.000000	B
B20	1.0	0.717598	0.588650	0.380490	Biso	1.000000	B
C1	1.0	0.320364	0.589059	0.382739	Biso	1.000000	C
C2	1.0	0.379596	0.339006	0.383468	Biso	1.000000	C
C3	1.0	0.320419	0.089057	0.382734	Biso	1.000000	C
C4	1.0	0.379598	0.838708	0.383459	Biso	1.000000	C
C5	1.0	0.399318	0.588809	0.383728	Biso	1.000000	C
C6	1.0	0.339704	0.339191	0.382949	Biso	1.000000	C
C7	1.0	0.399047	0.088815	0.383726	Biso	1.000000	C
C8	1.0	0.339705	0.838809	0.382951	Biso	1.000000	C
C9	1.0	0.498224	0.335764	0.384535	Biso	1.000000	C
C10	1.0	0.518879	0.088623	0.384479	Biso	1.000000	C
C11	1.0	0.498225	0.841521	0.384509	Biso	1.000000	C
C12	1.0	0.517002	0.588645	0.384549	Biso	1.000000	C
C13	1.0	0.577688	0.347644	0.384041	Biso	1.000000	C
C14	1.0	0.615359	0.444562	0.383462	Biso	1.000000	C
C15	1.0	0.615363	0.732695	0.383464	Biso	1.000000	C
C16	1.0	0.653657	0.348224	0.382423	Biso	1.000000	C
C17	1.0	0.675733	0.588618	0.381794	Biso	1.000000	C
C18	1.0	0.653666	0.829010	0.382418	Biso	1.000000	C
C19	1.0	0.671248	0.088624	0.381874	Biso	1.000000	C
C20	1.0	0.559760	0.088656	0.384212	Biso	1.000000	C
C21	1.0	0.555584	0.588671	0.384340	Biso	1.000000	C
C22	1.0	0.577696	0.829651	0.384050	Biso	1.000000	C
C23	1.0	0.458577	0.840110	0.384333	Biso	1.000000	C
C24	1.0	0.458578	0.337310	0.384369	Biso	1.000000	C
C25	1.0	0.439007	0.588734	0.384190	Biso	1.000000	C
C26	1.0	0.438780	0.088733	0.384181	Biso	1.000000	C
N1	1.0	0.100206	0.339245	0.381752	Biso	1.000000	N
N2	1.0	0.281502	0.589206	0.382337	Biso	1.000000	N
N3	1.0	0.221190	0.339404	0.382046	Biso	1.000000	N
N4	1.0	0.858255	0.339074	0.378268	Biso	1.000000	N
N5	1.0	0.979236	0.338773	0.379524	Biso	1.000000	N
N6	1.0	0.918735	0.088848	0.378525	Biso	1.000000	N
N7	1.0	0.039724	0.089030	0.380836	Biso	1.000000	N

N8	1.0	0.100206	0.839240	0.381752	Biso	1.000000 N
N9	1.0	0.281561	0.089204	0.382334	Biso	1.000000 N
N10	1.0	0.221190	0.839433	0.382049	Biso	1.000000 N
N11	1.0	0.858255	0.838631	0.378276	Biso	1.000000 N
N12	1.0	0.979236	0.838808	0.379524	Biso	1.000000 N
N13	1.0	0.918762	0.588848	0.378530	Biso	1.000000 N
N14	1.0	0.039721	0.589029	0.380834	Biso	1.000000 N
N15	1.0	0.160696	0.589472	0.382058	Biso	1.000000 N
N16	1.0	0.160696	0.089471	0.382059	Biso	1.000000 N
N17	1.0	0.737177	0.335901	0.379917	Biso	1.000000 N
N18	1.0	0.797899	0.088884	0.378716	Biso	1.000000 N
N19	1.0	0.737175	0.841515	0.379921	Biso	1.000000 N
N20	1.0	0.797600	0.588888	0.378740	Biso	1.000000 N