

Supporting Information

Tuning the Dirac Cone of Bilayer and Bulk Structure Graphene by Intercalating First Row Transition Metals using First Principles Calculations

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1 Detail Discussions of the Structure and Electronic Properties of the BLG-TM and bulk-BLG-TM (where TM: Fe-Zn)

The coordinates as well as electronic properties of the BLG and bulk-BLG materials were changed due to TM (TM: Fe, Co, Ni, Cu and Zn) intercalation. The equilibrium C-Fe bond distance and intercalation distance, d , of the BLG-Fe were increased by 0.009 Å and 0.024 Å respectively compared to the BLG-Mn. Similarly, the equilibrium bond and intercalation (d) distances were decreased in the bulk-BLG-Fe w.r.t. bulk-BLG-Mn; see Table 1. Similar trends were observed in the equilibrium C-Co, C-C bond distances and d for BLG-Co and bulk-BLG-Co w.r.t to the Mn-analogs. However, for both BLG-Co and bulk-BLG-Co, the bond distances and intercalation distance (d) were decreased in comparison to BLG-Fe and bulk-BLG-Fe. The electronic properties of Fe and Co atoms intercalated 2D layer structure BLG and bulk structure materials are shown in Figure 3f and in Figure 3g, respectively. The band structures and DOSs of BLG were changed due to the intercalation of Fe and Co atoms as the band structure calculations showed that the Dirac point is pushed down slightly from the E_F level by about 0.2 eV and 0.5 eV for BLG-Fe and BLG-Co, respectively, as depicted in Figure 3f and in Figure 3g, respectively. A large electron density appears around the E_F level in the total DOSs of the BLG-Fe due to the overlap of VB and CB below the Fermi level as depicted in the band structures and DOSs calculations. These calculations reveal that graphene features are dominant and the p orbital electrons of carbon are providing the large electron density around the E_F level whereas the d -orbital electrons of the Fe have negligible contribution in the total DOSs as shown in the right hand side of Figure 3f. Interestingly, the present DFT calculations found that the BLG-Co showed semi-metallic behavior like graphene, with the VB and CB overlapping into each other, but the total DOSs calculations show that the electron density is close to zero at the E_F level (see Figure 3g), similar to monolayer graphene. To put in another way, the total DOSs follows the p -orbital electron density character of C atoms in graphene, while the d -orbitals have negligible contribution, giving rise to BLG-Co as a semi-metal. The band structures and DOSs calculations of the bulk-BLG-Fe and bulk-BLG-Co are shown in Figure 4f-g. The band structure calculations found that the bands are overlapped, and there is one band crossing point (Dirac point) at the K-point in both bulk-BLG-Fe and bulk-BLG-Co. These calculations indicate that the Dirac features still remains even when the TM atoms Fe and Co are intercalated in BLG. Electron density appears around the E_F level of both bulk-BLG-Fe and bulk-BLG-Co, and the projected DOSs calculations showed that d -orbitals of Fe and Co have less contribution in the total DOSs. Thus, the graphene features are going to dominate in bulk-BLG-Fe and bulk-BLG-Co, for which the total DOSs follow the same trend of p -orbital character from C. Interestingly, our DFT calculations found that VB and CB touch each other at the E_F , yielding a Dirac point at the H-point in BLG-Co. In other words, the graphene features are dominant around the

H-point in bulk-BLG-Co. This is consistent with the predictions that the bulk-BLG-Co is a Dirac material whereas BLG-Co is a semi-metal with zero band gap. The DOSs and sub-shells DOSs calculations revealed that p -orbital of carbon atoms in graphene dominate in BLG-Co, BLG-Fe, bulk-BLG-Co and bulk-BLG-Fe, i.e. they are providing the electron density around the Fermi level, while the d -orbitals of the TM (Co and Fe) have negligible contribution in the total DOSs around the E_F as depicted in Figure 8f-g and 9f-9g, respectively.

The C-Ni and d distances were increased in both BLG (2D) and bulk-BLG (3D) when BLG was intercalated with Ni atoms w.r.t BLG-Co and bulk-BLG-Co. The electronic properties calculations were carried out for BLG-Ni, bulk-BLG-Ni, BLG-Cu and bulk-BLG-Cu, to get their band structures and DOSs as shown in Figure 3h-i and 4h-i, respectively. The band structures found that the valence and conduction bands overlap on each other and the Dirac point was pushed down below the Fermi level at the K-point of both BLG-Ni and BLG-Cu. Our present computation reveals that the total DOSs of the BLG-Ni is about zero at the E_F , whereas BLG-Cu has large electron density around the E_F . The total DOSs follow the p -orbital character of C atoms in graphene resulting in the dominating graphene features observed in BLG-Ni (see the right hand side of Figure 3h). In the case of BLG-Cu, a large electron density appears in the total DOSs around the Fermi level resulting in a conductor due to the overlapping of VB and CB below the E_F at the K-point as depicted in Figure 3i. Electron density, which follows the p -orbital character of C atoms of graphene, occurs around the E_F , while there is no significant contributing components of the d -orbital electrons of the Ni as shown in Figure 3h. A large electron density appears in the total DOSs of BLG-Cu, and the DOSs calculations show that the p_z sub-shells of carbon provides the majority of the electron density around the Fermi level as depicted in Figure 8i. The present study reveals that BLG-Cu shows metallic behavior.

The band structures and DOSs of bulk-BLG-Ni and bulk-BLG-Cu are shown in Figure 4h and Figure 4i, respectively. The band structures and DOSs of bulk-BLG-Ni showed that VB and CB overlap around 1.1 eV above the Fermi level, while there is a large electron density around the E_F , consistent with a conductor (see Figure 4h). The band calculations showed that in bulk-BLG-Cu, the Dirac point appeared at the K-point; see Figure 4i. One Dirac point was moved above the E_F at K point and the other one moved down below the E_F in BLG-Ni, while the sub-shell electron density calculations reveals that the p_z sub-shells of carbon and d_{yz} sub-shells of Ni are providing the electron density around the E_F level as displayed in Figure 9h. In BLG-Cu, the Dirac point appeared in its band structures at the K-point and the other Dirac point moved down below the E_F level at the H-point as depicted in Figure 9i. Electron density was found around the E_F , which is due the contribution of electron density of p_z sub-shells of carbon as shown in Figure 9i. In both materials, the VB and CB are overlapped below the E_F level.

The equilibrium C-Zn bond and intercalation distances of both BLG-Zn and bulk-BLG-Zn were increased

in comparison with all other materials as reported in Table 1. The band structure and DOSs calculations of BLG-Zn and bulk-BLG-Zn are shown in Figure 3j and Figure 4j, respectively. The Dirac point at the K-point is pushed down below the E_F level and the total DOSs showed large electron distribution around the E_F of BLG-Zn due to overlap of valence and conduction bands; see Figure 3j. Similarly, the VB and CB of bulk-BLG-Zn overlap above the E_F level and the DOSs shows a relatively large population around it. The present DFT calculation reveals that the total density of states of both materials (bilayer and bulk structure) follow the p -orbital electron density due to Carbon, which also causes the large electron density around the Fermi level.

2 Optimized Structures of BLG-TM materials (.cif format)

The optimized structures are provided below in .cif format.

2.1 BLG-Sc: Sc Intercalated 2D Bilayer Graphene

```

data_BLG-Sc_2D_SLAB
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_symmetry_Int_Tables_number          191
_symmetry_cell_setting                hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  -x,-y,z
  y,-x+y,z
  x-y,x,z
  y,x,-z
  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
  -x,-y,-z
  y,-x+y,-z
  x-y,x,-z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
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  y,x,z
  x-y,-y,z
  -x,-x+y,z
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_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001  C      -0.33614 -0.16807  0.00377  0.00000  Uiso  1.00
C013  C       0.33333 -0.33333  0.00371  0.00000  Uiso  1.00
SC017 Sc      0.00000  0.00000  0.00000  0.00000  Uiso  1.00

```

2.2 BLG-Ti: Ti Intercalated 2D Bilayer Graphene

```

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_symmetry_equiv_pos_as_xyz
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  -y,x-y,z
  -x+y,-x,z
  -x,-y,z
  y,-x+y,z
  x-y,x,z
  y,x,-z
  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
  -x,-y,-z
  y,-x+y,-z
  x-y,x,-z
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  -y,x-y,-z
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  x-y,-y,z
  -x,-x+y,z
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_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
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C013  C       0.33333 -0.33333  0.00341  0.00000  Uiso  1.00
TI017 Ti      0.00000  0.00000  0.00000  0.00000  Uiso  1.00

```

2.3 BLG-V: V Intercalated 2D Bilayer Graphene

```

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  -y,x-y,z
  -x+y,-x,z
  -x,-y,z
  y,-x+y,z
  x-y,x,z
  y,x,-z
  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
  -x,-y,-z
  y,-x+y,-z
  x-y,x,-z
  x,y,-z
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_atom_site_occupancy
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C013  C       0.33333 -0.33333  0.00339  0.00000  Uiso  1.00
V017  V       0.00000  0.00000  0.00000  0.00000  Uiso  1.00

```

2.4 BLG-Cr: Cr Intercalated 2D Bilayer Graphene

```

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  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
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  -x,-y,-z
  y,-x+y,-z
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C013  C       0.33333 -0.33333  0.00331  0.00000  Uiso  1.00
CR017 Cr      0.00000  0.00000  0.00000  0.00000  Uiso  1.00

```

2.5 BLG-Mn: Mn Intercalated 2D Bilayer Graphene

```

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C013  C       0.33333 -0.33333  0.00358  0.00000  Uiso  1.00
MN017 Mn      0.00000  0.00000  0.00000  0.00000  Uiso  1.00

```

2.6 BLG-Fe: Fe Intercalated 2D Bilayer Graphene

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C013  C       0.33333 -0.33333  0.00344  0.00000  Uiso  1.00
FE017 Fe      0.00000  0.00000  0.00000  0.00000  Uiso  1.00

```

2.7 BLG-Co: Co Intercalated 2D Bilayer Graphene

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_atom_site_occupancy
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C013  C       0.33333 -0.33333  0.00342  0.00000  Uiso  1.00
C0017 Co      0.00000  0.00000  0.00000  0.00000  Uiso  1.00

```

2.8 BLG-Ni: Ni Intercalated 2D Bilayer Graphene

```

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  -x+y,y,-z
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  y,-x+y,-z
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  x-y,-y,z
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_atom_site_occupancy
C001  C      -0.33492 -0.16746  0.00351  0.00000  Uiso  1.00
C013  C       0.33333 -0.33333  0.00350  0.00000  Uiso  1.00
NI017 Ni      0.00000  0.00000  0.00000  0.00000  Uiso  1.00

```

2.9 BLG-Cu: Cu Intercalated 2D Bilayer Graphene

```

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loop_
_symmetry_equiv_pos_as_xyz
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  -y,x-y,z
  -x+y,-x,z
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  y,-x+y,z
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  y,x,-z
  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
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  -x,-y,-z
  y,-x+y,-z
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  x,y,-z
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  y,x,z
  x-y,-y,z
  -x,-x+y,z
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_cell_angle_alpha                     90.0000
_cell_angle_beta                      90.0000
_cell_angle_gamma                     120.0000
loop_
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_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001  C      -0.33500 -0.16750  0.00353  0.00000  Uiso  1.00
C013  C       0.33333 -0.33333  0.00349  0.00000  Uiso  1.00
CU017 Cu      0.00000  0.00000  0.00000  0.00000  Uiso  1.00

```

2.10 BLG-Zn: Zn Intercalated 2D Bilayer Graphene

```

data_BLG-Zn_2D_SLAB
_symmetry_space_group_name_H-M      'P6/MMM'
_symmetry_Int_Tables_number          191
_symmetry_cell_setting                hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  -x,-y,z
  y,-x+y,z
  x-y,x,z
  y,x,-z
  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
  -x,-y,-z
  y,-x+y,-z
  x-y,x,-z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  y,x,z
  x-y,-y,z
  -x,-x+y,z
_cell_length_a                        4.8988
_cell_length_b                        4.8988
_cell_length_c                        500.0000
_cell_angle_alpha                     90.0000
_cell_angle_beta                      90.0000
_cell_angle_gamma                     120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001  C      -0.33346 -0.16673  0.00578  0.00000  Uiso  1.00
C013  C       0.33333 -0.33333  0.00578  0.00000  Uiso  1.00
ZN017 Zn      0.00000  0.00000  0.00000  0.00000  Uiso  1.00

```

3 Optimized Structures of Bulk-BLG-TM Materials (.cif format)

The optimized structures are provided below in .cif format.

3.1 Bulk-BLG-Sc: Sc Intercalated Bulk Structure BLG

```

data_BLG-Sc_3D_Bulk_Graphite
_symmetry_space_group_name_H-M      'P6/MMM'
_symmetry_Int_Tables_number          191
_symmetry_cell_setting                hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  -x,-y,z
  y,-x+y,z
  x-y,x,z
  y,x,-z
  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
  -x,-y,-z
  y,-x+y,-z
  x-y,x,-z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  y,x,z
  x-y,-y,z
  -x,-x+y,z
_cell_length_a                        4.9861
_cell_length_b                        4.9861
_cell_length_c                        3.8001
_cell_angle_alpha                     90.0000
_cell_angle_beta                      90.0000
_cell_angle_gamma                     120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001  C      0.16850  0.33700  0.00000  0.00000  Uiso  1.00
C007  C      0.33333 -0.33333  0.00000  0.00000  Uiso  1.00
SC009 Sc     -0.00000  0.00000 -0.50000  0.00000  Uiso  1.00

```

3.2 Bulk-BLG-Ti: Ti Intercalated Bulk Structure BLG

```

data_BLG-Ti_3D_Bulk_Graphite
_symmetry_space_group_name_H-M      'P6/MMM'
_symmetry_Int_Tables_number          191
_symmetry_cell_setting                hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  -x,-y,z
  y,-x+y,z
  x-y,x,z
  y,x,-z
  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
  -x,-y,-z
  y,-x+y,-z
  x-y,x,-z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  y,x,z
  x-y,-y,z
  -x,-x+y,z
_cell_length_a                        4.9956
_cell_length_b                        4.9956
_cell_length_c                        3.4253
_cell_angle_alpha                     90.0000
_cell_angle_beta                      90.0000
_cell_angle_gamma                     120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001  C      0.16983  0.33967 -0.00000  0.00000  Uiso  1.00
C007  C      0.33333 -0.33333  0.00000  0.00000  Uiso  1.00
TI009 Ti     -0.00000  0.00000  0.50000  0.00000  Uiso  1.00

```

3.3 Bulk-BLG-V: V Intercalated Bulk Structure BLG

```

data_BLG-V_3D_Bulk_Graphite
_symmetry_space_group_name_H-M      'P6/MMM'
_symmetry_Int_Tables_number          191
_symmetry_cell_setting                hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  -x,-y,z
  y,-x+y,z
  x-y,x,z
  y,x,-z
  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
  -x,-y,-z
  y,-x+y,-z
  x-y,x,-z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  y,x,z
  x-y,-y,z
  -x,-x+y,z
_cell_length_a                        4.9909
_cell_length_b                        4.9909
_cell_length_c                        3.4500
_cell_angle_alpha                     90.0000
_cell_angle_beta                      90.0000
_cell_angle_gamma                     120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001  C      0.16872  0.33745 -0.00000  0.00000  Uiso  1.00
C007  C      0.33333 -0.33333 -0.00000  0.00000  Uiso  1.00
V009  V      -0.00000  0.00000  0.50000  0.00000  Uiso  1.00

```

3.4 Bulk-BLG-Cr: Cr Intercalated Bulk Structure BLG

```

data_BLG-Cr_3D_Bulk_Graphite
_symmetry_space_group_name_H-M      'P6/MMM'
_symmetry_Int_Tables_number          191
_symmetry_cell_setting                hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  -x,-y,z
  y,-x+y,z
  x-y,x,z
  y,x,-z
  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
  -x,-y,-z
  y,-x+y,-z
  x-y,x,-z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  y,x,z
  x-y,-y,z
  -x,-x+y,z
_cell_length_a                        4.9800
_cell_length_b                        4.9800
_cell_length_c                        3.4708
_cell_angle_alpha                     90.0000
_cell_angle_beta                      90.0000
_cell_angle_gamma                     120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001  C      0.16904  0.33809 -0.00000  0.00000  Uiso  1.00
C007  C      0.33333 -0.33333  0.00000  0.00000  Uiso  1.00
CR009 Cr     -0.00000  0.00000 -0.50000  0.00000  Uiso  1.00

```

3.5 Bulk-BLG-Mn: Mn Intercalated Bulk Structure BLG

```

data_BLG-Mn_3D_Bulk_Graphite
_symmetry_space_group_name_H-M      'P6/MMM'
_symmetry_Int_Tables_number          191
_symmetry_cell_setting                hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  -x,-y,z
  y,-x+y,z
  x-y,x,z
  y,x,-z
  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
  -x,-y,-z
  y,-x+y,-z
  x-y,x,-z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  y,x,z
  x-y,-y,z
  -x,-x+y,z
_cell_length_a                        4.9799
_cell_length_b                        4.9799
_cell_length_c                        3.5837
_cell_angle_alpha                     90.0000
_cell_angle_beta                      90.0000
_cell_angle_gamma                     120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001  C      0.16884  0.33769  0.00000  0.00000  Uiso  1.00
C007  C      0.33333 -0.33333 -0.00000  0.00000  Uiso  1.00
MN009 Mn      0.00000  0.00000 -0.50000  0.00000  Uiso  1.00

```

3.6 Bulk-BLG-Fe: Fe Intercalated Bulk Structure BLG

```

data_BLG-Fe_3D_Bulk_Graphite
_symmetry_space_group_name_H-M      'P6/MMM'
_symmetry_Int_Tables_number          191
_symmetry_cell_setting                hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  -x,-y,z
  y,-x+y,z
  x-y,x,z
  y,x,-z
  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
  -x,-y,-z
  y,-x+y,-z
  x-y,x,-z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  y,x,z
  x-y,-y,z
  -x,-x+y,z
_cell_length_a                        4.9733
_cell_length_b                        4.9733
_cell_length_c                        3.4230
_cell_angle_alpha                     90.0000
_cell_angle_beta                      90.0000
_cell_angle_gamma                     120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001  C      0.16899  0.33797 -0.00000  0.00000  Uiso  1.00
C007  C      0.33333 -0.33333 -0.00000  0.00000  Uiso  1.00
FE009 Fe      0.00000  0.00000 -0.50000  0.00000  Uiso  1.00

```

3.7 Bulk-BLG-Co: Co Intercalated Bulk Structure BLG

```

data_BLG-Co_3D_Bulk_Graphite
_symmetry_space_group_name_H-M      'P6/MMM'
_symmetry_Int_Tables_number          191
_symmetry_cell_setting                hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  -x,-y,z
  y,-x+y,z
  x-y,x,z
  y,x,-z
  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
  -x,-y,-z
  y,-x+y,-z
  x-y,x,-z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  y,x,z
  x-y,-y,z
  -x,-x+y,z
_cell_length_a                        4.9657
_cell_length_b                        4.9657
_cell_length_c                        3.3684
_cell_angle_alpha                     90.0000
_cell_angle_beta                      90.0000
_cell_angle_gamma                     120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001  C      0.16820  0.33639 -0.00000  0.00000  Uiso  1.00
C007  C      0.33333 -0.33333  0.00000  0.00000  Uiso  1.00
C0009 Co     -0.00000  0.00000  0.50000  0.00000  Uiso  1.00

```

3.8 Bulk-BLG-Ni: Ni Intercalated Bulk Structure BLG

```

data_BLG-Ni_3D_Bulk_Graphite
_symmetry_space_group_name_H-M      'P6/MMM'
_symmetry_Int_Tables_number          191
_symmetry_cell_setting                hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  -x,-y,z
  y,-x+y,z
  x-y,x,z
  y,x,-z
  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
  -x,-y,-z
  y,-x+y,-z
  x-y,x,-z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  y,x,z
  x-y,-y,z
  -x,-x+y,z
_cell_length_a                        4.9531
_cell_length_b                        4.9531
_cell_length_c                        3.4085
_cell_angle_alpha                     90.0000
_cell_angle_beta                      90.0000
_cell_angle_gamma                     120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001  C      0.16825  0.33650  0.00000  0.00000  Uiso  1.00
C007  C      0.33333 -0.33333 -0.00000  0.00000  Uiso  1.00
NI009 Ni     -0.00000 -0.00000 -0.50000  0.00000  Uiso  1.00

```

3.9 Bulk-BLG-Cu: Cu Intercalated Bulk Structure BLG

```

data_BLG-Co_3D_Bulk_Graphite
_symmetry_space_group_name_H-M      'P6/MMM'
_symmetry_Int_Tables_number          191
_symmetry_cell_setting                hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  -x,-y,z
  y,-x+y,z
  x-y,x,z
  y,x,-z
  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
  -x,-y,-z
  y,-x+y,-z
  x-y,x,-z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  y,x,z
  x-y,-y,z
  -x,-x+y,z
_cell_length_a                        4.9595
_cell_length_b                        4.9595
_cell_length_c                        3.4128
_cell_angle_alpha                     90.0000
_cell_angle_beta                      90.0000
_cell_angle_gamma                     120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001  C      0.16853  0.33705  0.00000  0.00000  Uiso  1.00
C007  C      0.33333 -0.33333  0.00000  0.00000  Uiso  1.00
CU009 Cu     -0.00000 -0.00000  0.50000  0.00000  Uiso  1.00

```

3.10 Bulk-BLG-Zn: Zn Intercalated Bulk Structure BLG

```

data_BLG-Zn_3D_Bulk_Graphite
_symmetry_space_group_name_H-M      'P6/MMM'
_symmetry_Int_Tables_number          191
_symmetry_cell_setting                hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  -x,-y,z
  y,-x+y,z
  x-y,x,z
  y,x,-z
  x-y,-y,-z
  -x,-x+y,-z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
  -x,-y,-z
  y,-x+y,-z
  x-y,x,-z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  y,x,z
  x-y,-y,z
  -x,-x+y,z
_cell_length_a                        4.8944
_cell_length_b                        4.8944
_cell_length_c                        5.7013
_cell_angle_alpha                     90.0000
_cell_angle_beta                      90.0000
_cell_angle_gamma                     120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001  C      0.16682  0.33364  0.00000  0.00000  Uiso  1.00
C007  C      0.33333 -0.33333  0.00000  0.00000  Uiso  1.00
ZN009 Zn     0.00000  0.00000 -0.50000  0.00000  Uiso  1.00

```