Supporting Information

Properties and Carrier Mobility of FeB$_2$ Monolayer: The Effects of Symmetry

Zijian Wang, a Ting Cheng, a,b,* and Zhirong Liu a,b,c*

a College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China.
b Center for Nanochemistry, Academy for Advanced Interdisciplinary Studies, Peking University, Beijing 100871, China
c State Key Laboratory for Structural Chemistry of Unstable and Stable Species, Beijing National Laboratory for Molecular Sciences, Peking University, Beijing 100871, China

* Corresponding Authors: Ting Cheng (chengting-cnc@pku.edu.cn), Zhirong Liu (LiuZhiRong@pku.edu.cn).

Table S1 Energies and magnetic properties with different $U_{\text{eff}}$. 

<table>
<thead>
<tr>
<th>$U_{\text{eff}}$ (eV)</th>
<th>$E_{\text{PBE} + u}$ (eV)</th>
<th>$E_{\text{HSE06}}$ (eV)</th>
<th>Total magnetic moment ($\mu_B$)</th>
<th>Local magnetic moment in Fe cations ($\mu_B$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-20.60788</td>
<td>-24.97730</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>1</td>
<td>-19.55811</td>
<td>-24.97535</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>3</td>
<td>-17.50953</td>
<td>-24.98386</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>5</td>
<td>-15.32429</td>
<td>-24.62538</td>
<td>1.508</td>
<td>1.728</td>
</tr>
</tbody>
</table>
FIG. S1 The band structures of FeB₂ monolayer by different $U_{\text{eff}}$ with spin-polarized.

The band structure of spin-up is showed by black lines and that of spin-down by red points. The blue dashed line represents the Fermi level and it has been set to 0 eV. (a) $U_{\text{eff}} = 0$ eV. (b) $U_{\text{eff}} = 1$ eV. (c) $U_{\text{eff}} = 3$ eV. (d) $U_{\text{eff}} = 5$ eV.

We test PBE + U ($U_{\text{eff}} = 0, 1, 3, 5$ eV) with spin-polarized calculations. (Table S1 and Fig. S1). It is clearly shown that FeB₂ monolayer is a non-magnetic when $U_{\text{eff}} = 0, 1, 3$ eV, while it becomes magnetic under $U_{\text{eff}} = 5$ eV. To determine the ground state of FeB₂ monolayer, we conduct HSE06 static calculation reading the electron densities and wave functions we got by PBE + U. The energy results (Table S1) shows that the HSE06 energy with wave functions of $U_{\text{eff}} = 3$ eV is the lowest. Therefore, $U_{\text{eff}} = 3$ eV is likely an appropriate choice and the FeB₂ monolayer is a non-magnetic in the ground state.

Moreover, from our calculation results, we found that this method will change the gap between VB and CB at Γ point from 3.73 eV ($U_{\text{eff}} = 0$ eV) to 4.08 eV ($U_{\text{eff}} = 3$ eV). But the Dirac cone at K point will not open, and the shape of band structures are very
similar. Besides, the Fermi velocity changes little [from $3.98 \times 10^5$ m/s ($U_{\text{eff}} = 0$ eV) to $4.31 \times 10^5$ m/s ($U_{\text{eff}} = 3$ eV)].

For HSE06 method, we obtained the band structure [Fig. S2(a)]. It can be seen that the shape of band structure is very similar with the result of PBE method and the Dirac cone still exists. The Fermi velocity is $6.20 \times 10^5$ m/s, and an intuitive contrast with PBE method is shown in Fig. S2(b) (We make the Dirac point coincidence and set it to 0 eV.) It is clear that the shape is the same, only the Fermi velocity of HSE06 is larger than that of PBE yet.

In conclusion, we think the FeB$_2$ monolayer is a non-magnetic system and Hubbard U does not have big effect on FeB$_2$ monolayer.

For the separation problem of projected wave function at Dirac point K. A circle centered on K whose radius were 2% of $\Gamma K$ as used to calculate projected wave function (Fig. S3). It is evident that for the k points near K, the total contribution of $d_{xz}$ and $d_{yz}$ is the same and less than the total contribution of $d_{xy}$ and $d_{x^2-y^2}$ which is also a constant.
A possible analyze is that, taking $d_{xz}$ and $d_{yz}$ as an example, the contributes of any orbit to the Dirac cones is constant

$$
VB(d_{xz}) + CB(d_{xz}) = C_1 \quad (S1)
$$

$$
VB(d_{yz}) + CB(d_{yz}) = C_1 \quad (S2)
$$

The above calculation results show that the contribution sum of the two orbitals in the conduction band or valence band is constant

$$
VB(d_{xz}) + VB(d_{yz}) = C_2 \quad (S3)
$$

$$
CB(d_{xz}) + CB(d_{yz}) = C_2 \quad (S4)
$$

where $C_1$ and $C_2$ are constant. From eqs. (S1)-(S4), we can only get $C_1 = C_2$, but we can’t uniquely solve the unknown terms. One possible form for the solution is

$$
\begin{align*}
VB(d_{xz}) &= CB(d_{yz}) = \frac{C_1}{2} + A\cos(\varphi) \\
VB(d_{yz}) &= CB(d_{xz}) = \frac{C_1}{2} - A\cos(\varphi)
\end{align*}
$$

(S5)
where $A, \varphi$ are arbitrary. The calculation of VASP can also only accurately determine the value of $C_1$. If it takes the form of the above (S5) solution, and the parameter selection of $\varphi$ is associated with the rotation angle of lattice basic vectors, we will get the result that the projected wave function will change with the rotation of the basic vectors. However, the parameter selection and even the form of the solution have randomicity, so the result has no chemical or physical meaning and cannot represent the real projected wave function of Dirac cones.

FIG. S4 The surface fitting for elastic constants $C_{12}$. The red balls are the data from VASP and blue surface is the fitting result.
FIG. S5 The band structure near the Dirac point. The balls are the data from VASP and surfaces are the fitting results. The black balls and blue surface are for the FeB$_2$ monolayer without any strains and the Fermi level is -4.73 eV. The yellow balls and pink surface are for the FeB$_2$ monolayer with -0.02 strains in armchair directions as an example and the Fermi level is -4.68 eV. The vacuum level is set to 0 eV.

From Fig. S5, it is clear that when under small stains, the Dirac cone of the FeB$_2$ monolayer will move while the gap won’t open, which agrees with the generalized deformation potential theory. The scattering data points from VASP calculation were subtracted the vacuum energy and then were fitted by the formula
\[ E(k_x, k_y) = E_0 \pm \hbar v_F \sqrt{(k_x - k_{F,x})^2 + (k_y - k_{F,y})^2} \]
with parameters \( E_0, v_F, k_{F,x}, k_{F,y} \) ( + for CB and – for VB). And \( E_0 \) gives the absolute \( E_{DP} \).
FIG. S6 The potential energy of graphene along the \( z \)-direction, where the plateaus corresponds to the vacuum energy.

The graphene is only one sheet, so its potential energy in vacuum is horizontal. (Fig. S6)

If we don’t use the dipole correction in VASP, the potential energy of \( \text{FeB}_2 \) monolayer is sloping, and the slope reflects the energy difference between two sides. (Fig. S7)

FIG. S7 The potential energy of \( \text{FeB}_2 \) monolayer without dipole correction.
FIG. S8 The potential energy of FeB$_2$ monolayer under different strains.

Under different strains, the slopes of the potential energy of FeB$_2$ monolayer under...
different strains are different. (Fig. S8) And the slope is linear with the distances between Fe and B sheet, which also shows the accuracy of the parallel plate capacitor model. (Fig. S9)