Electronic Supplementary Material (ESI) for RSC Advances.

the supplemental information

Tuning the electronic and magnetic properties of penta-graphene by using hydrogen atom: a theoretical study

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xyz coordinates of the M-PG system

M-PG

1.00000000000000

3.6418411732000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 3.6418411732000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 14.8981475830000001

C H

6 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.1333333402648407	F	F	F
0.5063852271889999	0.4936340638130332	0.1334009758717443	T	T	T
0.3713427554244291	0.1269500030726221	0.0934166026962586	T	T	T
0.6335949660677684	0.8646921598744797	0.0934082233893463	T	T	T
0.1501643157341590	0.6434546514751176	0.1875438461454735	T	T	T
0.8630893054211484	0.3562386496954701	0.1788079300943508	T	T	T
0.2280995891746898	0.7220778489712885	0.2564283652329493	T	T	T

xyz coordinates of the WM-PG system

WM-PG

1.00000000000000

3.6418411732000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 3.6418411732000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 14.8981475830000001

C H

6 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.1333333402648407	F	F	F
0.5072959346623359	0.4929059452055385	0.1333978325703331	T	T	T
0.3716893767638944	0.1266642377685214	0.0935348584992923	T	T	T
0.6338383833388567	0.8645032609538230	0.0935271523525327	T	T	T
0.1500938887586558	0.6429818530219454	0.1876660027212440	T	T	T
0.8633348107751255	0.3560992844810484	0.1785466403541442	T	T	T
0.2282041840795452	0.7223486956989560	0.2564569206659971	T	T	T

The methodology to obtain the STM images

It works like this:

1) Relax.

2) Calculate CHGCAR and W***ECAR for the relaxed structure.

3) Generate PARCHG --- partial density charge using the CHGCAR and W***ECAR.

PARCHG has the same format as CHGCAR. It is a density for a certain energy range.

It is calculated by setting LPARD=.TRUE.

The decisive parameters are NBMOD and EINT.

If NBMOD=-3 (the most sensible setting), then EINT contains an energy interval with respect to Fermi energy, for which the partial density will be evaluated.

For more details, see the pardens.F file.

Thus, the typical setup for generating PARCHG for STM is:

LPARD=.TRUE.

NBMOD=-3

EINT=-0.1 0.1

(plus other standart INCAR settings)

As soon as you have PARCHG, you can calculate the STM images either by showing one plane of the PARCHG (constant distance mode) or showing some isosurface (constant current mode).

In our group an utility th_stm was used together with the data explorer (www.opendx.org).

However, I just finished working on the STM applet for p4vasp and it will be released soon (maybe this week).

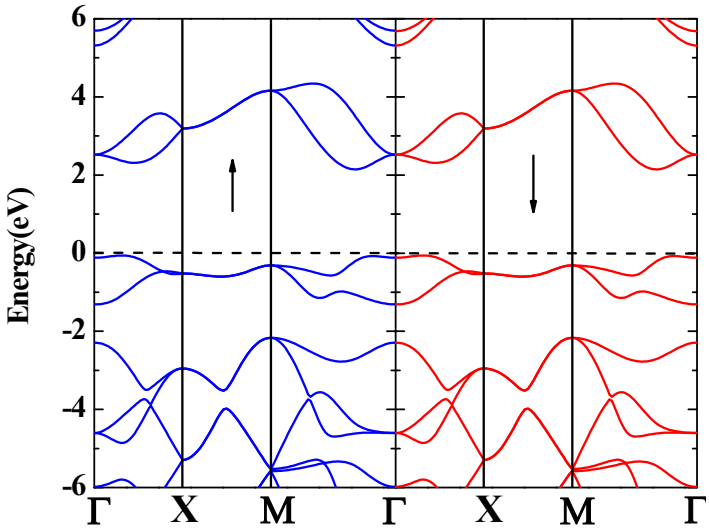

Fig. S1 Electronic band structure of the PG sheet. The arrow denotes the spin-polarized direction. The Fermi level is shifted to 0 eV.

Electronic band structures for PG sheet is depicted in Fig. S1. It is seen that the calculated band gap of PG is around 2.22 eV, which is in excellent agreement with 2.24 eV of B. Rajbanshi et al.[1] The Fermi level is set at 0 eV. The paired spin-up and spin-down channels of the band structures imply that the PG is still a nonmagnetic sheet. The energy of sub-VBM on the M-Γ path is very close to that of the true VBM on the Γ-X path, and the CBM is located on the M-Γ path, thus PG can be considered as a quasi-direct-band-gap semiconductor.

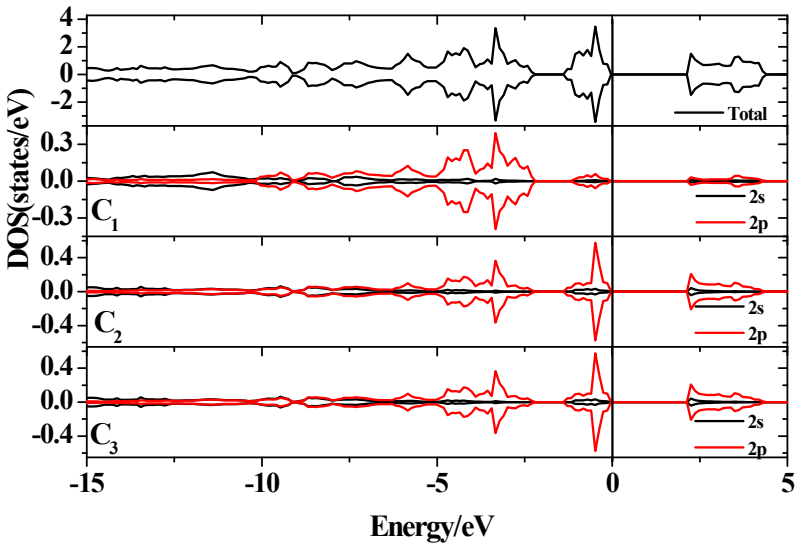

Fig. S2 The spin-polarized LDOS of the PG sheet. The positive and negative LDOS denote the spin-up and spin-down states, respectively. The vertical dashed line indicates the Fermi level.

The spin-polarized LDOS of the PG sheet shown in Fig. S2. The electronic states near the Fermi level primarily originate from the sp^2 hybridized C_2 and C_3 atoms. And the spin-up and spin-down DOS of the C_1, C_2, C_3 orbitals and the total DOS are symmetric and induce no magnetic moments.

1. B. Rajbanshi, S. Sarkar, B. Mandal and P. Sarkar, *Carbon*, 2016, **100**, 118-125.