Negative differential resistance, perfect spin filtering effect and tunnel magnetoresistance in vanadium-doped zigzag blue phosphorus nanoribbons

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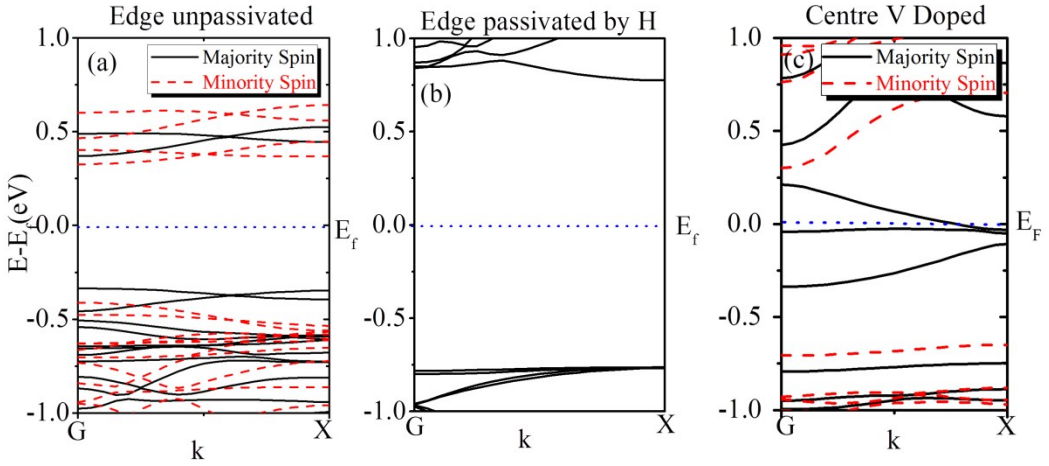
For NDR

For our blue phosphorene nanoribbons system, the presence of vanadium is the cause of the negative differential resistance of zigzag blue phosphorene nanoribbons (zBPNRs).

The band structure of H-saturated zBPNRs show the nonpolarization semiconductor properties in the Figs. 1(b), there is no bands near the Fermi lever. So when we add the bias into the passivated device and there is no negative differential resistance effect.

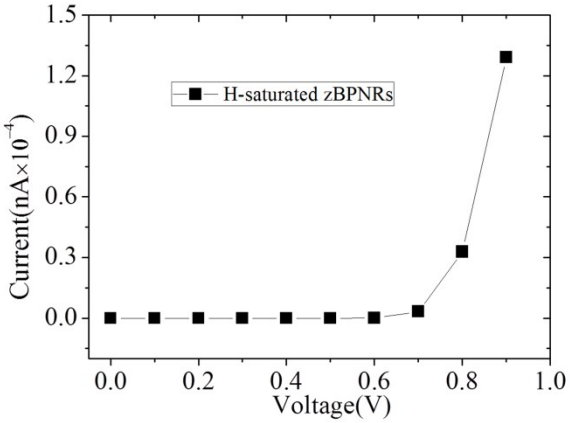
Also, we calculated band structure of the edge unpassivated zBPNRs in Figs 3(a), showing the magnetic semiconductor properties. There are some bands distributed near the energy 0.5ev and -0.5eV. And there is no negative differential resistance effect, too.

So in our system, there are three bands near the Fermi lever in Figs.1(c). The NDR is mainly caused by the three hybrid energy bands. So, the presence of vanadium is the cause of the negative differential resistance of zBPNRs and it is not the inherent in nanoribbons themselves.



Figs. 1 Calculated band structure of (a) edge unpassivated, (b) edge passivated by H and (c) V centre-doped 12-zBPNR.

We also calculate the IV curve of H-saturated zBPNRs, showing the rapidly increasing current by increasing voltage. And there is no negative differential resistance effect.



Figs. 2 I–V curves of the leads for the H-saturated zBPNRs.

For MPSH

In our calculations, the MPSH – The molecular projected self-consistent Hamiltonian. The MPSH states are obtained by diagonalizing the molecular part of the full self-consistent Hamiltonian.

The transmission eigenvalues are obtained by diagonalizing the transmission matrix. The number of eigenvalues indicates the number of individual channels through the molecule, and the eigenvalue shows the strength of each channel. The eigenvalues are the true transmission probabilities, and thus lie in the interval [0, 1]. If several channels are available at a particular energy, their sum - and hence the transmission coefficient at this energy - may however be larger than 1. Most of the eigenvalues are very small and can be neglected. The two largest eigenvalues of each energy are the most important ones.

We would now like to project the transmission eigenstate onto the MPSH states of the doped blue phosphorus nanoribbons (zBPNRs), to find the orbitals that carry the transmission.

The scattering state is expanded in basis orbitals, $\phi_i(r)$ through

$$\psi(r) = \sum_i v_i \phi_i(r),$$

We now diagonalize the self consistent Hamiltonian projected onto zBPNRs,

$$H^{zBPNRs} c_\alpha = \varepsilon_\alpha S^{zBPNRs} c_\alpha,$$

where *c* are the expansion coefficients of the MPSH states.

Next we can expand the projection of the scattering state of the zBPNRs molecule in the MPSH states, through

$$v = \sum_{\alpha} a_{\alpha} c_{\alpha},$$

where the expansion coefficients are given by $a_{\alpha} = c_{\alpha}^{\dagger} S^{\mathrm{zBPNRs}} v.$ Through the magnitude of each a_{α} we can get the relevance of each MPSH state, and

$$\sum_{\alpha} |a_{\alpha}|^2 = v^{\dagger} S^{\mathrm{zBPNRs}} v.$$

Below is given a script that calculates the largest eigenvalue scattering state and calculates the projection weight of each MPSH state

$$p_{\alpha} = \frac{|a_{\alpha}|^2}{v^{\dagger} S^{DTB} v}.$$

1. S.-C. Zhu, C.-T. Yip, S.-J. Peng, K.-M. Wu, K.-L. Yao, C.-L. Mak, C.-H. Lam, Half-metallic and magnetic semiconducting behaviors of metal-doped blue phosphorus nanoribbons from first-principles calculations, *Phys. Chem. Chem. Phys.* 2018, **20**, 7635.