

Magnetic properties of tilted phosphorene nanoribbon under electric field

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Study on phosphorene nanoribbon was mostly focused on zigzag and armchair structures and no ferromagnetic ground state was observed in these systems. Here, we investigated the magnetic property of tilted black phosphorene nanoribbons (TPNRs) affected by an external electric field. We also studied the edge passivation effect on the magnetism and thermal stability of the nanoribbons. The pure TPNR displayed an edge magnetic state, but it disappeared in the edge reconstructed TPNR due to the self-passivation. In addition, we found that the bare TPNR was mechanically unstable because an imaginary vibration mode was obtained. However, the imaginary vibration mode disappeared in the edge passivated TPNRs. No edge magnetism was observed in hydrogen and fluorine passivated TPNRs. In contrast, the oxygen passivated TPNR was more stable than the pure TPNR and the edge-to-edge antiferromagnetic (AFM) ground state was obtained. We found that the magnetic ground state could be tuned by the electric field from antiferromagnetic (AFM) to ferromagnetic (FM) ground state. Interestingly, the oxygen passivated TPNR displayed a half-metallic state at a proper electric field in both FM and AFM states. This finding may provoke an intriguing issue for potential spintronics application using the phosphorene nanoribbons.

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