

Manipulation of magnetic state in armchair black phosphorene nanoribbon by charge doping

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Using the first principles studies, we investigated the width dependent magnetic properties of armchair black phosphorene nanoribbons (APNRs) by controlling the electron charge doping. In the unrelaxed APNRs the antiferromagnetic coupling between two phosphorus atoms in the same edge was found. However, the edge magnetic moment vanished after structure relaxation, and all the APNRs showed a semiconducting feature. Interestingly, the charge doping substantially altered the band structures of the APNRs because the metallic states reappeared in the charge doped APNRs. Besides, the magnetic moment was found in the charge doped systems. We found that the Stoner condition could nicely explain the magnetic moment at the edge atoms. Moreover, we propose that the edge-to-edge magnetic coupling can be manipulated by charge doping because the transition from antiferromagnetic to ferromagnetic state was achieved. Our findings may bring interesting issues for spintronics applications.

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