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2D Materials and Devices for Spintronics: First-principles Studies

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The key to success of spintronics is identification of suitable materials and evaluation of their performance in devices. While experimental studies take time and require a lot of resources, computational study, particularly the first-principles calculations, is playing an important role. We have been using such methods to investigate a series of materials as well as conceptual design of spintronic devices.

In earlier studies, [1,2] we proposed spin logic gates based on zigzag graphene nanoribbons. However, some issues still remain for graphene based spintronic devices, and one of them is the low efficiency of spin-injection from a metal lead to graphene. Through first-principles calculations, we found that spin injection efficiency from a metal lead to graphene can be enhanced by using a hexagonal boron nitride (*h*-BN) between the electrode and graphene. The minority-spin-transport channel of graphene can be strongly suppressed by the insulating *h*-BN barrier, resulting in a high spin-injection efficiency. This is due to asymmetric effects of the barrier on the two spin states of graphene. [3]

We also investigated transport property of phospherene nanoribbons (PNRs). In contrast to graphene and MoS_2 nanoribbons, the carrier transport channels under low bias are mainly located in the interior of both armchair and zigzag PNRs, and immune to small amounts of edge defects. A PNR-based dual-gate field-effect transistor, with high on/off ratio of 10^3, was proposed based on the giant electric-field tuning effect. [4]

Our recent calculations reveal that phospherene can be made magnetic by an interplay of vacancy and strain, even though neither P vacancy nor external strain alone results in magnetism in phosphorene. When either a biaxial strain or a uniaxial strain along the zigzag direction of phosphorene containing P vacancies reaches 4%, the system favors a spin-polarized state with a magnetic moment of 1 μ_B per vacancy site. This is due to spin-polarized p states of under-coordinated P atoms next to the vacancy, which are bonded in the absence of the external strain or when phosphorene is subjected to a low strain. [5]

References:

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