

Spin polarized bands in 2D materials Silicene and MoS₂

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Abstract

Spintronics has drawn tremendous attention in the past decade because of the high potential for the spin transport electronics in the next generation semiconductor industry as well as for the future quantum computing. One of the core topics in the spintronics is how to efficiently generate the spin current of nearly 100 % spin polarization. Earlier efforts concentrated on searching for magnetically doped semiconductors and half-metallic materials such as CrO₂, Fe₃O₄, SrRuO₃, and so on, in which only one spin channel is conducting with the other insulating. To date however most of the half-metals are magnetic materials and a large part of them are transition-metal oxides, making the applications on nowadays semiconductor industry difficult. Consequently controllable non-magnetic spintronic devices are highly desirable in the development of spintronics applications, which is an area of intense current interest. We predict that field-gated silicene possesses two gaped Dirac cones exhibiting nearly 100 % spin-polarization, situated at the corners of the Brillouin zone by using first-principles calculations. Consequently a silicene-based spin-filter should enable the spin-polarization of an output current to be switched electrically without external magnetic fields. On the other hand, we predicted by using first-principles calculations that MoS₂ exhibits intrinsic spin splittings in the conduction band maximum due to the spin-orbit interaction at the K-point in the Brillouin zone of the honeycomb-like structure. These spin polarized bands have been observed in spin-polarized ARPES measurements by our collaborators recently.