Theory and modelling of low dimensional materials

Hashmi Arqum

Ultrafast Dynamics Group, QST

Abstract

Due to the extraordinary physical and electronic properties of materials with reduced dimensionality is considered as the most promising candidate to replace silicon in future electronic devices. In practical, magnetic semiconductors will allow us to control charge as well as quantum spin state. But up to date, all 2D materials like graphene, transition metal chalcogenides, phosphorene etc. lack magnetism. The reduction of dimensionality has increased the possibility of actualization of spin related phenomena. A key challenge, a stimulating innovation in this area, is the generation of 100% spin-polarized currents at the Fermi level. In the present work, we use the efficiency of density functional theory to unravel the electronic and magnetic structures of promising candidates of 2D materials. Particularly, our focus is 2D magnetic semiconductors which will enable us to make multi-functional, flexible, and transparent nano-devices.

hashmi.arqum@qst.go.jp