Ab initio calculation of intrinsic spin-Hall effect in graphene nanostructures

BIN WANG, JIAN WANG, Department of Physics, The University of Hong Kong, Pokfulam Road, Hong Kong, China, HONG GUO, Center for the Physics of Materials and Department of Physics, McGill University, Montreal, PQ, Canada H3A 2T8 — We report a theoretical analysis of intrinsic spin-Hall effect in a four-probe graphene nanostructure in the absence of spin orbit interaction and magnetic field. The nanostructure consists of a finite size graphene sheet connected to the outside world by two zigzag graphene nano-ribbons (ZGNR) and two armchair graphene nano-ribbons (AGNR), forming a cross-shaped two-dimensional device. Due to edge states induced magnetism at ZGNR boundaries, our result suggests that a pure spin-current without an accompanying charge current, is intrinsically induced giving rise to a spin-Hall effect. We have calculated the spin-Hall conductance by an atomic first principles method where density functional theory is carried out within the Keldysh nonequilibrium Green’s function framework.