SPIN-RESOLVED STM SIMULATION OF GRAPHENE NANORIBBON

Wei Ji[1,2], *Werner A. Hofer*[3], *Hong-Jun Gao*[2], *and Hong Guo*[1]
Centre for the Physics of Materials and Department of Physics, McGill University, Montreal, Quebec, Canada H3A 2T8
Department of Chemistry, The University of Liverpool, Liverpool L69 LBX, UK
Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China
wei.ji@mcgill.ca

Graphene nanoribbon was predicted by previous literature to exhibit ferromagnetic magnetism at its zig-zag edge and anti-ferromagnetic coupling between the two edges of the ribbon [1]. Spin-polarized scanning tunneling spectroscopy (SPSTM) may be able to experimentally verify this prediction. In this work, we report a calculated spin contrast in SPSTM setup from atomic first principles. Using a DFT based scattering states method [2], we calculate a series of SPSTM images of grapheme nanoribbons having zig-zag edges. A free-standing ribbon, a ribbon on a free-standing two dimensional graphene sheet, and a ribbon on a SiC(0001) supported (C terminated) two dimensional grapheme sheet, have been investigated. It was found that the spin-contrast at zig-zag edges should be detectable. The contrast can also be enhanced or suppressed by interlayer interactions of graphene ribbon and the graphene sheet underneath.

References:

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