Origin of edge magnetism in zig-zag graphene nanoribbons

JEIL JUNG, ALLAN MACDONALD, University of Texas at Austin — We explore the physical origins of edge magnetism in zig-zag terminated graphene nanoribbons addressing the role of exchange effects and the band structure in the ferromagnetic alignment of the spins along the edge, the preference of anti-ferromagnetic inter-edge ground state to the ferromagnetic one, and the microscopic physics of the spin stiffness along an edge. Our analysis of the qualitative physics will rest largely on unrestricted Hartree-Fock theory calculations for π-band model Hamiltonians with long-range Coulomb interactions. Unlike Hubbard models, or ab initio LDA calculations, this type of theory can consistently account for non-local exchange effects.

Jeil Jung
University of Texas at Austin

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