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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 interedge 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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