

Abstract Submitted
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Edge Magnetism in Graphene Nanoflakes¹ TANUSRI SAHA-DASGUPTA, S.N.Bose National Centre for Basic Sciences, MUKUL KABIR, Indian Institute of Science, Education and Research, Pune, India — We will discuss the manipulation of magnetism in small sized hexagonal graphene nanoflakes. We explore possible ways to manipulate the intrinsic edge magnetism in hexagonal graphene nanoflake with zigzag edges, using density functional theory supplemented with on-site Coulomb interaction. The effect of carrier doping, chemical modification at the edge, and finite temperature on the edge magnetism has been studied. The magnetic phase diagram with varied carrier doping, and on-site Coulomb interaction is found to be complex. Chemical modification of the edge atoms by hydrogen leads to partial quenching of local moments, giving rise to a richer phase diagram. We further report the influence of temperature on the long-range magnetic ordering at the edge using ab initio molecular dynamics. These findings will have important implications in controlling magnetism in graphene based low dimensional structures for technological purpose, and in understanding varied experimental reports.[*]

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