

Abstract Submitted
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Controlling Adatom Magnetism on Bilayer Graphene by External Field MUKUL KABIR, Indian Institute of Science Education and Research, Pune 411008, India, DHANI NAFDAY, TANUSRI SAHA-DASGUPTA, S. N. Bose National Centre for Basic Sciences, Kolkata 700098, India — We study the effect of external electric field on the magnetic properties of single Fe adatom and Fe dimer hosted on a bilayer graphene surface grown on a SiO₂ substrate within first-principles calculations. We find that electric field perpendicular to the bilayer graphene modulates the charge and spin-state of the single Fe adatom over a wide range. States ranging from $3d^6$, S=2 to $3d^{10}$, S=0 have been observed for Fe adatom, which may be inaccessible under normal condition. This would be of interest in the context of orbitally controlled Kondo effect. Further, for Fe-dimer, we find that a small electric field is able to tune the magnetic exchange coupling. Interestingly, we also observe an unusual magnetostructural coupling for Fe-dimer, which stabilizes a ferrimagnetic state over a fully compensated antiferromagnetic spin configuration.

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