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Magnetism of Adatom on Bilayer Graphene and its Control: A First-principles Perspective[1] TANUSRI SAHA-DASGUPTA, DHANI NAFDAY, S.N.Bose National Centre for Basic Sciences — We present first-principles investigation of the electronic and magnetic properties of adatom on bilayer graphene within the framework of density functional theory. In particular, we study the influence of an applied gate-voltage which modifies the electronic states of the bilayer graphene as well as shifts the adatom energy states relative to that of the graphene energy states. Our study carried out for a choice of three different adatoms, Na, Cu and Fe, shows that the nature of adatom-graphene bonding evolves from ionic to covalent, in moving from alkali metal, Na to transition metal, Cu or Fe. This leads to the formation of magnetic moments in the latter cases (Cu, Fe) and its absence in the former (Na). Application of an external electric field to bilayer graphene, completely changes the scenario, switching on a magnetic moment for Na adatom, and switching off the magnetic moments for Cu, and Fe adatoms. Our results have important implications for fundamental studies of controlled adatom magnetism and spintronics application in nanotechnology.

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