The Electric Field Effect on the Chemisorption of Cu Atom on Perfect Graphene

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ABSTRACT

The influence of an external static electric field on the chemisorption of a single Cu atom on perfect graphene (Cu/graphene) is explored and investigated using magnetic moment and electronic structure calculations based on the Anderson model, which is characterized by various model parameters. The Cu atom on top of a carbon atom site configuration is taken into account in our research. The effects of an electric field on Cu chemisorption on graphene were examined. The changes in charge accumulation on the adatom Cu confirm the potential of altering the magnetic characteristics of Cu/graphene via the perpendicular electric field direction. The magnetic moment on Cu/graphene was measured as a function of the electric field. Metallic state is observed for multiple electric field values on a single Cu adatom/graphene with variable electronic structure. It has been discovered that the bonding between Cu atoms and graphene can be tuned using an electric field. The dependence of adatom/graphene electronic and magnetic properties on the density of states indicates the importance of the microscopic details for graphene functionalization towards spintronics applications. Our findings could be quite interesting since they imply that the magnetic moment and spin dependent electronic structure on the Cu atom site can be modified by the electric field action.

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