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Geometric stabilities, electronic and magnetic properties of stable palladium adsorption on graphene – A first principle study

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Abstract

There have been continuing efforts simultaneously to explore the effects of various adsorbed guest atoms or molecules on graphene because potential applications and electronic transports properties experiments with graphene require contact with metal electrodes. Research interests in transition metal adsorption expand the ranges of applications from catalysis, spintronics to magnetic device. In this work, geometric stabilities, electronic and magnetic properties of low-coverage stable palladium (Pd) adsorbed graphene are studied based on first principles plane wave implemented in the QUANTUM ESPRESSO simulation package. It is found that single Pd adsorbing on top of carbon atom site is the most stable configuration. Moreover, the study reveals that the graphene with single Pd atom is metallic and non-magnetic. For palladium dimer, it is found that, depending on the configuration of the parallel or perpendicular Pd, two distinct situations with respect to magnetic behavior can be realized. For parallel configurations where the bonding is more strengthened, Pd dimer adsorbing on top of two carbon atoms site is the favored configuration and non-magnetic. Furthermore, the study also reveals that in spite of low coverage Pd dimer adsorbed graphene the system is metallic. This further reveals the possibility of using palladium atom on graphene for catalytic hydrogen storage. For perpendicular Pd configurations, reasonable magnetic moment was detected for depending on the strength of the Pd-graphene bond. These results demonstrate that the graphene electronic and magnetic properties can be effectively modified by Pd dimer metal adsorption and this may serve as a potential material in nanodevices applications.

Biography

Md Mahmudur Rahman has completed his Ph.D from Osaka University, Japan. He is presently a Senior Lecturer in Department of Physics, Universiti Putra Malaysia. His main research interest is theoretical and computational solid state physics and material science. He has published about 30 papers in reputed journals.