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

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There have been continuing efforts simultaneously to explore the effects of various adsorbed guest atoms or molecules ongraphene because potential applications and electronic transports properties experiments with graphene require contact withmetal 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 stablepalladium (Pd) adsorbed graphene are studied based on first principles plane wave implemented in the QUANTUMESPRESSO simulation package. It is found that single Pd adsorbing on top of carbon atom site is the most stableconfiguration. Moreover, the study reveals that the graphene with single Pd atom is semiconductingand non-magnetic. For palladiumdimer, 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 dimeradsorbing on top of two carbon atoms site is the favored configuration and non-magnetic. Furthermore, the study also revealsthat in spite of low coverage Pd dimer adsorbed graphene the system is metallic. This further reveals the possibility of usingpalladium atom on graphene for catalytic hydrogen storage. For perpendicular Pd configurations, reasonable magneticmoment was detected for depending on the strength of the Pd-graphene bond. These results demonstrate that the grapheme electronic and magnetic properties can be effectively modified by Pd dimer metal adsorption and this may serve as a potentialmaterial 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.

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