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研究论文



# 铜族金属与完整及氮掺杂石墨烯的相互作用

尹伟1, 林华香2, 章永凡1, 黄昕1, 陈文凯1,2,*

1福州大学化学系, 福建福州 350116; 2福州大学福建省光催化重点实验室—省部共建国家重点实验室培育基地, 福建福州 350002

YIN Wei1, LIN Huaxiang2, ZHANG Yongfan1, HUANG Xin1, CHEN Wenkai1,2,?

1Department of Chemistry, Fuzhou University, Fuzhou 350116, Fujian, China; 2Fujian Provincial Key Laboratory of Photocatalysis, State Key Laboratory Breeding Base, Fuzhou University, Fuzhou 350002, Fujian, China

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摘要 基于广义梯度密度泛函理论和周期平板模型, 研究了铜族金属单原子和双原子簇与完整及氮掺杂石墨烯的结合情况. 结果表明, 氮掺杂后石墨烯的电子结构特性由半金属性变为金属性; 铜族金属在完整及石墨型氮掺杂石墨烯上的吸附较弱, 结合能约为 0.5 eV, 而在吡啶型氮掺杂和吡咯型氮掺杂石墨烯上有较强的化学吸附, 结合能一般大于 1 eV; 吡咯型氮掺杂后的构型不稳定, 金属原子及簇与包含该结构的石墨烯衬底作用时会使其向吡啶型氮掺杂转变, 并最终得到基于吡啶型氮掺杂的稳定吸附构型. Mulliken 电荷布居分析显示, 吸附在吡啶型氮掺杂石墨烯上的金属单原子与金属双原子簇带电性质相反. 态密度及轨道分析表明, Cu 与吡啶型氮掺杂石墨烯空位处留有悬挂键的三个原子成键, 而 Au 与其中两个 C 原子成键.

关键词: 密度泛函理论 铜族金属 氮掺杂 石墨烯 吸附

Abstract: The binding strength of coinage metal (IB group) single and double atoms clusters on perfect or N-doped graphene has been studied with the periodic slab model using generalized gradient approximation (GGA). The calculated results indicated that N-doped graphene showed metallic electron properties rather than semimetallic ones of perfect graphene. Physical or weak chemical adsorption was got on perfect or graphite N-doped graphene with the binding energy around 0.5 eV. Chemical adsorption happened on pyridine N-doped graphene and pyrrole N-doped graphene with binding energy above 1 eV. Pyrrole N-doped graphene was less stable than graphite N-doped graphene or pyridine N-doped graphene. When adsorbates interacted with pyrrole N-doped graphene, it carried out the transition from pyrrole N-doped graphene to pyridine N-doped graphene, and the most stable adsorption structure based on pyridine N-doped graphene was obtained finally. The analysis of Mulliken population indicated that metal single atoms had positive charge while double atom clusters had negative charge after adsorbing on pyridine N-doped graphene. The density of states and orbital analysis demonstrated that Cu atom bonded with three atoms with dangling bonds while Au atom bonded with two of them in pyridine N-doped graphene.

Keywords: density functional theory, coinage metal, N-doping, graphene, adsorption

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