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A DFT investigation of CO adsorption on VIIIB transition metal-doped graphene sheets

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ABSTRACT

Adsorptions of CO on pristine, Fe-, Ru-, Os-, Co-, Rh-, Ir-, Ni-, Pd-, and Pt-doped graphene were investigated, using density functional theory calculation at B3LYP/LanL2DZ theoretical level. This work revealed that the transition metal doped graphenes were more highly sensitive to CO adsorption than that of pristine graphene. The Os- and Fe-doped graphenes displayed the strongest interaction with C and O atoms of CO molecule, respectively.

1. Introduction

Graphene is a novel nanomaterial in which a single atomic layer of graphite is formed in a hexagonal lattice. Since the first synthesis via a "Scotch tape" method of graphene sheets was reported in 2004 [1–3], graphene has been one of the most active research fields. Potential applications of graphene in integrated circuits, transparent conducting electrodes, hydrogen storage materials, solid-state gas sensors, and biosensors have been widely explored since its discovery [2–5]. Recently, it has been reported that graphene-based systems may also be used as excellent gas sensor [6–9]. A major limitation for future applications of graphene-based gas sensor is that the pristine graphene is rather chemically inert due to the strong sp^2 binding between carbon atoms in the graphene plane. Thus, the interaction between graphene and the reaction center is quite weak. Some other recent theoretical studies [10–13] proposed that transition metal doping in graphene might significantly enhance the

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chemical reactivity and improve the electronic structure of the system, suggesting a great potential of this material for future application in gas sensor.

Gas sensing is very important in environmental issues, and much research has focused on the development of suitable gas-sensitive material and hazardous chemical removal [14–16]. During the past decade, graphene surfaces have been the subject of tremendous activity and investigation for use in hydrogen storages [17,18], gas sensors [19,20] and lithium-ions storage [21]. To date, the adsorption of several molecules on their surface has been investigated, such as CO [7], NH_3 [7], NO [7,8], NO_2 [7,8], O_2 [8], CO_2 [9], CH_2O [22], CH_4 [23], $C_9H_{10}N_2O_5$ [24], and HCN [25]. One of the gases which have been extensively studied is CO gas because it is known to be extremely harmful to the human body, and it is also a main cause of air pollution. CO adsorptions on the surface of nanotube, such as pristine boron nitride nanotube (BNNT) [26], boron phosphide nanotube [26], aluminum phosphide nanotube [26], carbon nanotube [27], and aluminum nitride nanotube [26,28] were investigated and reported. The N- [29] and Pd-doped [30] single wall carbon nanotube (SWCNT) present high sensitivity toward CO, compared with the pristine SWCNT. The CO molecule displays strong chemical interaction with Ni-doped BNNTs, compared to the pristine tubes [31]. Apart from nanotube, graphene sheet is the one of nanomaterials used as CO adsorption. Several works reported that the adsorption ability of CO molecule on graphene sheet is improved by metal doping [32–34]. Previous experimental studies have shown that graphenes supported palladium can efficiently adsorb the CO molecule [32]. The Al-doped graphene boron nitride sheet has strong chemisorption of CO molecule, where CO adsorbed onto pristine graphene remains a weak interaction [33]. Theoretical studies have shown that the Cu-, Ag-, and Au-doped graphenes can significantly enhance its adsorption ability with CO gas [33].

However, the interactions of CO molecule adsorbed on the VIIIB transition metals (TM)-doped graphene sheets have not been investigated. Therefore, in the present work, our main objective is to study the CO adsorption behavior of VIIB TM atoms doped graphene sheets including Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, and Pt atoms.

2. Computational details

The graphene sheet model composed of 42 carbon and 18 hydrogen atoms (Fig. 1(a)) which is nearly the same size of model reported in many previously works, was chosen for this study [7,8,10,12,13,16,20–25]. Hydrogen atoms were used to saturate the carbon atoms with dangling bonds at the edge of graphene sheet. The Fe-, Ru-, Os-, Co-, Rh-, Ir-, Ni-, Pd-, and Pt-doped graphene sheets

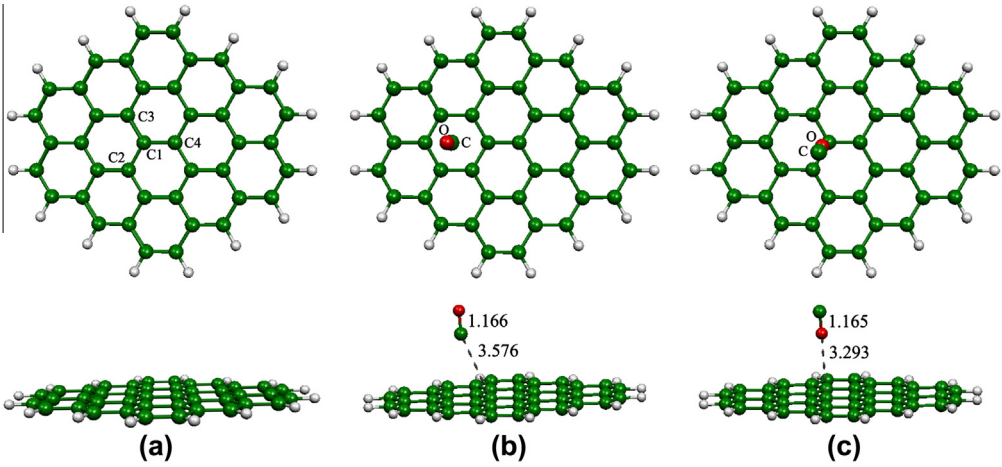

Fig. 1. The B3LYP/LanL2DZ optimized structures of the (a) graphene sheet, (b) CO adsorbed on graphene sheets as configurations of CO when pointing its C atom toward the adsorption site, and (c) CO adsorbed on graphene sheets as configurations of CO when pointing its O atom toward the adsorption site. Bond distances are in Å.