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REGULAR ARTICL

Spin polarization properties of benzene molecule adsorbed at Fe(100) surface: first principles calculations

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Abstract: Based on density functional theory (DFT), the spin polarization properties of a benzene molecule which is adsorbed at Fe (100) surface are discussed. A variety of horizontal and vertical adsorption configurations as well as their influences on the spin density distributions is detailed studied. It is found that the interfacial orbital hybridization occurred between the 3d orbital of Fe atoms and the 2p hybridized orbital of carbon atoms. The appearance of the new interfacial coupling state make the two spin state near Fermi level no longer equal to each other. After adsorbed at Fe (100) surface, the benzene molecule is no longer spin degeneracy, an obvious spin polarization appeared. It is also found that the interfacial spin polarization for the horizontal adsorption is bigger than that of the vertical adsorption. The biggest spin polarization will be obtained when the center of the benzene ring is directly placed above the Fe atom.

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1. Introduction

In the past few decades, a significant progress in the study of organic semiconductors is their applications in spintronics. Organic semiconductors have weak spin orbit coupling and weak hyperfine interactions, which are contributed to the spin polarized injection and transportation. Due to the size diversity and the variety of organic molecules, it is possible to

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produce high quality and low cost information equipments. Based on organic molecular devices, the study of its spin injection, spin polarized transportation, spin storage and spin detection have become hot topics in today's research field of spintronics[1-4].

The properties of ferromagnetic/organic interface and its influence on the device functionalities have attracted people's interest in organic spintronics[5-16]. In 2002, Dediu *et al.* used $La_{0.3}Sr_{0.7}MnO_3$ (LSMO) as spin polarized electron donors and they studied the spin polarized injection and transportation in the structure of LSMO/T6/LSMO system[5]. Xiong *et al.* made an organic spin valve device of Co/Alq3/LSMO in 2004, in which the magnetic resistance reached to 40% at low temperature[6]. From then on, people widely studied the properties of organic magnetic devices both theoretically and experimentally. The influence of different electrodes, different organic materials and different external conditions on the spin polarization properties as well as the mechanisms are discussed[7]. For example, Sun *et al*. studied the adsorption properties of pentacene on the Fe(100) surface experimentally and theoretically.The spin density distributions and the plane-averaged density of states at the vacuum side are computed, from which they concluded that the spin polarization is negative at the donated molecular orbital and positive at the back donated orbital close to the Fermi level[8,9]. Nicolae Atodiresei *et al.* designed the local spin polarization by adsorbing organic molecules contain $\pi(p_z)$ electrons onto a magnetic surface[10]. Souraya Goumri-Said *et al*. investigated the spin polarization at the interface between Fe(100) and a benzene for two positions of the organic molecule, which is planar and perpendicular respecting to the substrate[11]. Xuhui Wang *et al*. investigated the spin polarization properties at the interface between a thiophene molecule and Co substrate by using the ab initio calculations. They found that the reduced symmetry in the thiophene molecule leads to a strong spatial dependence of the spin polarization[12]. Ding Yi *et al.* also selected some typical adsorption configurations in benzene/Co system to reveal the spin polarization properties by using first-principles calculations [13].

In experiments, the molecular beam epitaxial and chemical vapor deposition methods are usually used to fabricate organic devices, so there are randomness between the organic molecules and metal electrode contacts. On the other hand, there are plenty of experimental evidences had already showed that the organic molecules can be spin polarized when they are adsorbed to the metal contacts, and also the spin polarization properties can be modified by changing the different contact configurations[14-16]. Therefore, it is interesting to make clear why the different adsorption configurations can affect the spin polarization properties between the organic molecules and the ferromagnetic contacts. In this article, benzene molecule/Fe electrode organic component is selected as the model system to study the interface spin polarization properties. The benzene molecule is one of the most popular small organic molecules which are used in the research field of spinterface[17-25].