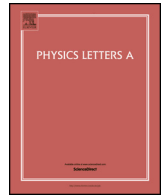




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Multiple spin-resolved negative differential resistance and electrically controlled spin-polarization in transition metal-doped [6]cycloparaphenylenes

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ABSTRACT

In structure, a [n]cycloparaphenylene ([n]CPP) molecule is constructed by fully conjugated bent benzenes, i.e., hexangular rings. Based on first-principles calculations, the spin-dependent electronic transport of transition metal-doped CPP, X@[6]cycloparaphenylene (X@[6]CPP) (X=Fe, Co and Ni), contacted with Au electrodes is investigated. (Multiple) negative differential resistance (NDR) is observed for all the doping cases, suggesting it is the intrinsic feature of such systems. Due to the spin dependence of the NDR, electrical switch of the direction of spin polarization for a current is realized. Further analysis shows that it is the suppression of the transmission peaks around the Fermi level as the bias increases that results in the NDR. The suppression is caused by the decay of the local density of states on the scattering region. As electrically controlled spin polarization is a promising area in nanoelectronics, we believe our results would be quite beneficial to the development of spintronic devices.

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1. Introduction

In recent years, spintronics has become a promising field in nanoelectronics [1–3]. Due to the demand of reducing dimensions of electronic devices, lots of attention has been paid to molecular spintronics, where molecules are used as spin transport channels. Up to now, tremendous (spin-related) electronic phenomena have been revealed in molecular systems, such as spin filter effect and negative differential resistance (NDR) [4–10]. Among them, NDR attracts much attention owing to the wide application potentials, e.g., memory, amplification and logic operator [5–11].

Due to the peculiar electrical properties, carbon-based structures are considered to be one of the most promising materials for future nanoelectronic devices [12]. Recently, the synthesis of [n]cycloparaphenylene ([n]CPP) has attracted great interest because of its unique geometry [13–15]. In structure, a [n]CPP molecule is constructed by several fully conjugated bent benzenes, i.e., hexangular rings. For instance, [6]CPP is made up of 6 benzenes [16,17].

For hexangular ring-based carbon structures, great progress has been made in spintronics, especially in graphene and carbon nanotubes [18–20]. To fulfill the gap of their application in molecular spintronics, there is a need to explore the spin-dependent electronic properties in hexangular ring-based molecules. Owing to the geometry, [n]CPP becomes a good candidate. However, unlike zigzag graphene ribbons, there is no zigzag edge on this molecule, so it does not possess spontaneous magnetism. Thus, although much attention has been paid to the synthesis and electronic structure of [n]CPPs, few of them focus on the spin-related electronic transport.

As well known, doping is a useful way to modulate the electronic structure and transport properties in nanomaterials. Furthermore, doping with transition metal could make a system acquire magnetism and exhibit interesting spin-related features [21–29]. In the present work, we investigate the spin-dependent transport of [6]CPP systems doping with transition metals, i.e., X@[6]CPP (X=Fe, Co and Ni), which are contacted with Au electrodes. The study is carried out by density functional theory calculations (DFT) combined with nonequilibrium Green's function (NEGF). It is found that Fe- and Co-doped systems exhibit spin-polarized transport and Ni-doped ones exhibit spin-unpolarized transport. Moreover,

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1 NDR phenomenon is observed in all doping systems (multiple
2 NDRs for some cases), suggesting it is the intrinsic feature of such
3 systems. In Fe- and Co-doped cases, NDR exhibits spin asymmetric
4 dependence. This results in a switch of the direction for the
5 spin polarization of the current, realizing the control of spin polar-
6 ization through electrical means. Electrically controlled spin polar-
7 ization is a promising area in nanoelectronics, as compared with
8 conventional magnetic ways, it could reduce the energy consump-
9 tion and dimensions of the devices [30,31]. We believe our results
10 is quite useful in the development of spintronic devices.

12 2. Computational method

14 The calculations are carried out using the Atomistix Toolkit
15 package [32–34], which is based on the combination of DFT and
16 NEGF. We use the mesh cutoff energy of 150 Ry, and $1 \times 1 \times 100$
17 k -point mesh in the Monkhorst–Pack scheme [35]. The Perdew–
18 Burke–Ernzerhof formulation of the generalized gradient approxi-
19 mation (GGA) to the exchange correlation functional is used [36].
20 The double-zeta polarized (DZP) basis set of local numerical or-
21 bitals is employed in all the calculations. The supercell with suf-
22 ficient vacuum spaces (more than 10 Å) is chosen to prevent the
23 interactions with adjacent images. To mimic the actual situation,
24 the positions of all atoms in the configurations have been re-
25 laxed before the transport calculations and the maximal force is
26 set to be 0.02 eV/Å. According to previous experimental and theo-
27 retical studies on related systems, such a kind of carbon-based
28 molecule could remain its structure after contacting with metal
29 electrode, which has been confirmed by the optimization calcula-
30 tions based on density functional theory [37,38]. In the present
31 work, the molecule-electrode distance is optimized by minimizing
32 the total energy of the two-probe system. This contact method
33 has been widely used in the two-probe systems based on metal-
34 molecule-metal configurations [39,40].

35 In NEGF theory, the current is obtained according to the
36 Landauer–Büttiker formula

$$37 I(V)_{\uparrow\downarrow} = \frac{2e}{h} \int T(E, V)_{\uparrow\downarrow} [f(E - \mu_L) - f(E - \mu_R)] dE,$$

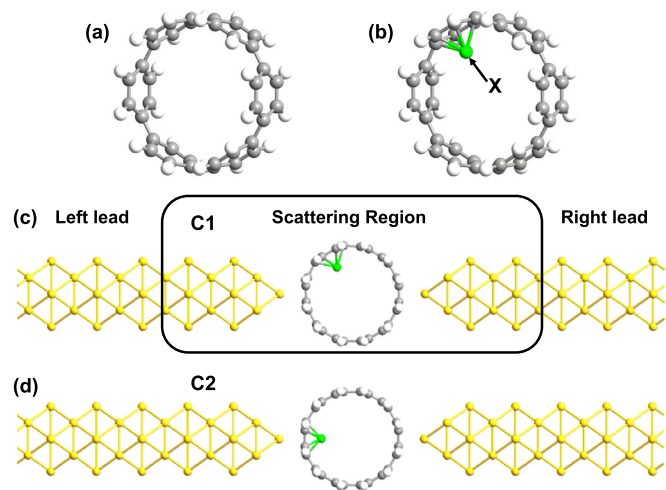
38 where $\mu_{L/R}$ is the chemical potential of the left/right electrode,
39 $f(E - \mu_{L/R})$ is the Fermi function of the left/right electrode, and
40 $V = (\mu_L - \mu_R)/e$ is the bias window. In theory, the bias window is
41 defined as the integral window for calculating the current. In the
42 present work, it refers to $[E_F - V/2, E_F + V/2]$, where E_F is the
43 quasi Fermi level of the two-probe system. $T(E, V)_{\uparrow\downarrow}$ is the trans-
44 mission probability through the system for spin-up/down, which is
45 obtained by (the denotation of spin is omitted)

$$46 T(E, V) = Tr[\Gamma_L(E, V)G^R(E, V)\Gamma_R(E, V)G^A(E, V)],$$

47 where $G^{R/A}(E, V)$ is the retarded/advanced Green's function of the
48 scattering region, and $\Gamma_{L/R}$ is the coupling matrix to the left/right
49 electrode.

52 3. Results and discussions

53 In structure, [6]CPP can be considered as a nano hoop consisting
54 of six fully conjugated bent benzenes in the para position, shown
55 in Fig. 1(a). The molecule is saturated with H atoms on the edges
56 to eliminate dangling bonds. In experiment, [6]CPP could be syn-
57 thesized in at least two ways [16,17]. As we know, there are many
58 ways of doping in such a molecule. Here the CPP molecule is like
59 a cage. Doping the metal atom on the inner site and exposing
60 carbon atoms outside would make the configuration be more inert,
61 compared with that exposing the metal atom outside. It is
62 quite beneficial for the practical application, which would make



67 Fig. 1. (Color online.) (a)–(b) The structures of pristine [6]CPP and X@[6]CPP, re-
68 spectively. X = Fe, Co and Ni. (c)–(d) Geometries of the two-probe Au–X@[6]CPP–Au
69 systems for contact configurations of C1 (c) and C2 (d), respectively.
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the nanoelectronic devices possess good stabilization. In addition,
previous studies show that, for transition metals, hollow site is
more favorable for doping in such a kind of system [41–43]. So,
in the present work, we focus on the inner hollow site of the ring
to dope with transition metals. Here, we choose Fe, Co and Ni to dope
in [6]CPP on the inner hollow site of the ring, shown in Fig. 1(b)
(X@[6]CPP, X = Fe, Co and Ni). To mimic the realistic situation,
Au nanowire with an atomic tip is used as the electrode to study the
transport properties, which is contacted with the molecule on its
hollow site. To realize a good contact between the molecule and
electrodes, we contact the Au electrodes at the hollow site of the
molecule. In a [6]CPP molecule, there are six hexagonal rings. So,
there will be totally six two-probe contact configurations. Consider-
ing the symmetry of the left and right electrodes, as well as the
symmetry of the doping molecule, there is only two independent
contact configurations, i.e., C1 and C2, shown in Fig. 1(c) and (d)
respectively. Other contact configurations are equivalent to them.
For configuration C1, the rings contacted with electrodes are not
doped with metal atoms. And for configuration C2, there is a rota-
tion of the molecule compared with that of C1, and the ring doped
with metal atom contacts with the left electrode. So, the difference
between C1 and C2 is the orientation of the molecule relative to
the electrodes.

Fig. 2 shows the total and spin-resolved currents as a function
of the bias voltage (I – V curve) for Fe-doped systems (Fe@[6]CPP),
where the left and right panels are for the configurations of C1
and C2 respectively. For configuration C1, one easily finds there is
a threshold at the bias of 0.8 V. The total current increases only
a little when the bias is smaller than 0.8 V, see Fig. 2(a). Actually,
there is a NDR in the bias region of [0.4, 0.6] V, but not obvious.
When V_b is larger than 0.8 V, the current increases almost linearly
with V_b . However, when V_b exceeds 1.7 V, the current decreases
with the further increase of bias and the NDR behavior appears
again.

From the spin-resolved I – V curves in Fig. 2(b), one finds the
spin-up and down currents show the same variation trend as the
total one in Fig. 2(a). But they are not the same between spin-up
and down, so the current becomes spin-polarized. For the spin-
up current, there are two main NDR regions, i.e., [0.4, 0.6] V and
[1.7, 2.0] V (note there is an oscillation around 1.9 V). However,
for spin-down one, there is only one NDR region around 1.8 V, and
there is none in the lower bias range of [0.4, 0.6] V. As the total
current is the sum of the spin-up and down currents, the NDRs

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