This is an Accepted Manuscript, which has been through the Royal Society of Chemistry peer review process and has been accepted for publication.

Accepted Manuscripts are published online shortly after acceptance, before technical editing, formatting and proof reading. Using this free service, authors can make their results available to the community, in citable form, before we publish the edited article. We will replace this Accepted Manuscript with the edited and formatted Advance Article as soon as it is available.

You can find more information about Accepted Manuscripts in the Information for Authors.

Please note that technical editing may introduce minor changes to the text and/or graphics, which may alter content. The journal’s standard Terms & Conditions and the Ethical guidelines still apply. In no event shall the Royal Society of Chemistry be held responsible for any errors or omissions in this Accepted Manuscript or any consequences arising from the use of any information it contains.
Effects of 3d transition-metal doping on electronic and magnetic properties of MoS₂ nanoribbons

Xiaoqing Tian, Lin Liu, Yu Du, Juan Gu, Jian-bin Xu, and Boris I. Yakobson

Received (in XXX, XXX) Xth XXXXXXXXX 20XX, Accepted Xth XXXXXXXXX 20XX
DOI: 10.1039/b000000x

The electronic and magnetic properties of MoS₂ nanoribbons doped with 3d transitional metals (TMs) were investigated using first-principles calculations. Clean armchair MoS₂ nanoribbons (AMoS₂NRs) are nonmagnetic semiconductors whereas clean zigzag MoS₂ nanoribbons (ZMoS₂NRs) are metallic magnets. The 3d TM impurities tend to substitute the outermost cations of AMoS₂NRs and ZMoS₂NRs, which are in agreement with the experimental results reported. The magnetization of the 3d-TM-impurity-doped AMoS₂NRs and ZMoS₂NRs is configuration dependent. The band gap and carrier concentration of AMoS₂NRs can be tuned by 3d-TM doping. Fedoped AMoS₂NRs exhibit ferromagnetic characteristics and the Curie temperature ($T_C$) can be tuned using different impurity concentrations. Co-doped ZMoS₂NRs are strongly ferromagnetic with a $T_C$ above room temperature.

15 Introduction

The MoS₂ monolayer is composed of three covalently bonded hexagonal atomic layers (S–Mo–S). Weak van der Waals interactions exist between adjacent MoS₂ monolayers. One important advantage of MoS₂ is that the electronic and optical properties can be tuned by varying the number of layers. The bulk MoS₂ crystal is an indirect gap semiconductor with a band gap of 1.29 eV, whereas the MoS₂ monolayer is a direct gap semiconductor with a band gap of 1.90 eV. One-dimensional MoS₂ has been synthesized in recent experiments. Quasi-1D nanotubes and nanoribbons of MoS₂ share the honeycomb structure and are expected to display interesting electronic and magnetic properties arising from quantum confinement effects. Defects and strain are expected to modify the electronic properties and magnetic of MoS₂ monolayer and nanoribbons. MoS₂ nanostructures are doped with 3d TMs such as Fe, Co, and Ni to increase its catalytic activities in hydridesulfurization processes in the oil industry. The magnetic and electronic properties of MoS₂ nanoribbons could be tuned by 3d TMs doping. Either 3d TM substrates or 3d TM nanoclusters could alter the electronic structures of MoS₂ monolayer. We used state-of-the-art first-principles technique to study the electronic and magnetic properties of 3d TMs (including Mn, Fe, and Co)-doped MoS₂ nanoribbons with armchair- and zigzag-shaped edges.

40 Computational methods

Theoretical calculations were performed with the Quantum Espresso package, employing the GGA-PBE exchange correlation functional. The on-site Coulomb interaction GGA+U for 3d TMs is used. The U and J are the on-site Coulomb repulsion and exchange interaction parameters, respectively. Typical values of U and J are 4.0 and 1.0 eV, respectively, for both Mn and Fe; for Co, U and J are 3.3 and 1.0 eV. 40 Ry is used as the plane-wave basis set cutoff. The structural models of MoS₂ nanoribbons are constructed by cutting a single-layered MoS₂ with the desired edges and widths. The 1-D periodic boundary condition was applied along the growth direction of the nanoribbons to simulate infinitely long nanoribbon systems; the length scales for the MoS₂ nanoribbons are defined in Ref. 5. Specifically, the width of AMoS₂NRs is defined by the number of dimmer columns whereas for ZMoS₂NRs it is defined by the number of Mo columns. A 1.6-nm-thick vacuum layer was used to eliminate longitudinal interactions between the super cells. For the 14-AMoS₂NR, the
super cell contains in total 168 atoms, and its in-plane size is around 3.5 nm (width)×2.2 nm, which is large enough to avoid lateral image interactions. For 10-ZMoS$_2$NR, the super cell contains in total 120 atoms, and its in-plane size is around 4.0 nm (width)×0.7 nm, which is also large enough to avoid lateral image interactions. A sampling of 12 uniformly distributed k-points along the 1-D Brillouin zone is employed for the MoS$_2$ nanoribbons for both the zigzag and armchair shaped edges.

Results and discussion
10 The structures of relaxed 14-AMoS$_2$NRs (Fig. 1(a)) give a width of around 2.1 nm. After structural optimization, the width of 14-AMoS$_2$NR is increased by around 1.5 percent. There is obvious structural reconstruction to mitigate the truncation of chemical bonds at the edges. The S–Mo bonds in MoS$_2$ are composed of partial covalent and ionic bonds similar to the bonds of ZnO. The oxidation state of the edgiest Mo is +1.63, which is 0.1 smaller than that of the interior Mo using the Bader analysis method$^{20}$ The edgiest Mo atom is moved by 0.3 Å inwards relative to the edgiest S atom. The bond length of S–Mo bond is about 0.1 Å smaller than that of the interior bond. The calculated spin-polarized density of states (SPDOS) of 14-AMoS$_2$NR (Fig. 1(b)). The 14-AMoS$_2$NR is a nonmagnetic semiconductor with band gaps of 0.56 eV and this is in good agreement with Ref. 5. The band gap value is determined by the difference in the on-site energies of two edges, and intra- and inter-edge hopping parameters of the tight-binding models.$^{21}$ Because clean 14-AMoS$_2$NR is a nonmagnetic semiconductor, 3d TMs (Mn, Fe, Co) are used as dopants to achieve magnetic properties. Seven substitution sites are considered (Fig. 1(a)) with impurity concentrations corresponding to 1.79 percent. Substituted by 3d TM-doped 14-AMoS$_2$NRs for the seven configurations. 3d TM-impurity-doped 14-AMoS$_2$NRs exhibit obvious configuration-dependent formation energies and electronic and magnetic properties. Their formation energies are calculated from

$$\Delta H_f(TM) = E_{tot}(TM) - E_{tot}(clean) - \sum_i n_i \mu_i,$$

where $E_{tot}(TM)$ is the total energy of the doped 14-AMoS$_2$NR and $E_{tot}(TM)$ the total energy of the undoped 14-AMoS$_2$NR. $\mu_i$ denotes the chemical potential for species $i$ (host atoms or dopants), and $n_i$ the corresponding number that have been added or removed from the supercell.

For 3d TM-doped 14-AMoS$_2$NR, configuration 1 has the lowest formation energy (Fig. 1(c)), and hence is the most favored. Configuration 4 has the highest formation energy, so is the least favored. The 3d TM impurities tend to replace the outermost cations. The order of the formation energies is $H_f(Mn) < H_f(Fe) < H_f(Co)$. This can be attributed to size effects of the 3d dopants; the larger the atomic radius of the dopant, the closer it is to the host Mo atom and thus the lower the formation energy. From the configuration-dependent magnetic moment of the 3d TM impurities (Fig. 1(d)), the magnetic moments of the impurities in configuration 1 for the 3d TM-impurity-doped 14-AMoS$_2$NRs, are larger than those of other configurations. Mn, Fe, and Co impurities of configuration 1 have local magnetic moments of 3.3, 2.5, and 0.9 Bohr magneton ($\mu_B$), respectively. Similarly, Mn, Fe, and Co adatoms on the MoS$_2$ monolayer have local magnetic moments of 3.0, 2.0, and 1.0 $\mu_B$, respectively.$^{22}$
where $E_{AF}$ and $E_{FM}$ are the total energies of the AFM and FM state, respectively. The $\Delta E$ is 21 meV for the Fe-impurity-pair-doped 14-AMoS$_2$NRs with configuration $\alpha$, so the FM state is more stable than the AFM state. The magnetic exchange coupling of configuration $\beta$ gave a $\Delta E$ of 11 meV which is 10 meV smaller than that of configuration $\alpha$. There exists FM coupling between the Fe impurity pairs. We further increased the on-site Coulomb repulsion interaction $U$ to 5 and 6 eV and found that $\Delta E$ was almost unchanged. The Ruderman–Kittel–Kasuya–Yosida interaction could be the origin of the ferromagnetism. The magnetic exchange interactions between the 3d TM impurities in Heisenberg model is written as:

$$H = -2JS_1 \cdot S_2,$$

(3)

where $J$ is the magnetic exchange coupling between neighboring magnetic atoms; $S_1$ and $S_2$ are the spins of the magnetic atoms 1 and 2. The total spin of the atom is given by $S = (N_\uparrow - N_\downarrow)/2$, here $N_\uparrow$ and $N_\downarrow$ are the numbers of spin-up and spin-down electrons, respectively. According to eqns (2) and (3), the magnetic exchange coupling is obtained from $J = \Delta E/(4S_1S_2)$. Here each Fe has a local magnetic moment of 2.5 $\mu_B$. Thus we can take $S = S_1 = S_2 = 1.25$. Based on these values, the magnetic exchange coupling $J$ is 3.36 meV for Fe-doped 14-AMoS$_2$NR with configuration $\alpha$. The critical temperature $T_C$ as estimated using the mean field method is

$$T_C = \frac{2S(S+1) \Delta E}{3k_B J} = \frac{(1 + \frac{1}{S}) \Delta E}{6k_B},$$

(4)

where $\Delta E$ is 30, 15, and 22 meV for the Fe-impurity-pair-doped 10-, 12- and 14-AMoS$_2$NRs, respectively in configuration $\alpha$ giving a corresponding $T_C$ of 104, 52, and 76 K calculated using eqn (4).

**Table 1** Summary of $\Delta E$ (meV) for 3d TM impurity-doped AMoS$_2$NRs of different widths. $\alpha$ and $\beta$ refer to configurations $\alpha$ and $\beta$, respectively

<table>
<thead>
<tr>
<th>Width</th>
<th>$\alpha$</th>
<th>$\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>30</td>
<td>15</td>
</tr>
<tr>
<td>12</td>
<td>21</td>
<td>11</td>
</tr>
<tr>
<td>14</td>
<td>22</td>
<td>13</td>
</tr>
<tr>
<td>16</td>
<td>23</td>
<td>18</td>
</tr>
</tbody>
</table>

Here the calculated $T_C$ is 73 K. From the magnetic exchange coupling for Fe-pair-doped AMoS$_2$NRs of different widths (see Table 1), $\Delta E$ is 30, 15, and 22 meV for the Fe-doped 10-, 12- and 14-AMoS$_2$NRs, respectively in configuration $\alpha$ giving a corresponding $T_C$ of 104, 52, and 76 K calculated using eqn (4).
The $\Delta E$ is 10, 8, and 13 meV for the Fe-doped 10-, 12-, and 16-AMoS$_2$NRs, respectively, in configuration $\beta$ giving a corresponding $T_C$ of 35, 28, and 45 K. For these AMoS$_2$NRs, the $T_C$ associated with configuration $\alpha$ is higher than that for configuration $\beta$. As indicated in Fig. 2(c), the magnetization of a doped 14-AMoS$_2$NR is mainly distributed on the Fe pair, and the Mo atoms along the doped edge have opposite magnetization directions to Fe. The edge states contribute mainly to the magnetization and occupy the electronic orbitals near the Fermi level. Thus the edge states are more active and dominate the physical properties of AMoS$_2$NRs. Compared with clean 14-AMoS$_2$NRs, the band gap of the Fe-pair-doped 14-AMoS$_2$NR has been obviously reduced. Based on Fig. 2(d), the band-gap values are 0.35 and 0.29 eV for the spin-up (majority) and spin-down (minority) bands, respectively. The blue shifts of the band gaps of 14-AMoS$_2$NR have been obviously reduced. Based on Fig. 2(d), the band-gap values of 0.01, and 0.20 eV, respectively. This will enhance the local concentration of 3.57 percent will lift up the Fermi level by 0.09, 0.01, and 0.20 eV, respectively. This will enhance the local concentration of Fe impurities; the $T_C$ of Fe-doped 14-AMoS$_2$NR is far above room temperature.

Based on the SPDOS (Fig. 2(f)), the band gap of spin-up and spin-down bands is 0.18 and 0.26 eV, respectively, so the band gap has been further reduced by increasing the concentration of Fe impurities.

The temperature-dependent magnetic moment can be estimated from the Stoner and spin-fluctuation models,$^{26}$

$$M = M_0 \left[ 1 - \left( \frac{T}{T_C} \right)^2 \right]^\frac{1}{2},$$

$$M = M_0 \left[ 1 - \left( \frac{T}{T_C} \right)^2 \right]^\frac{1}{2},$$

where $M_0$ is the magnetization of the ground state. The $M_0$ of each Fe impurity of doped 14-AMoS$_2$NR, with structure shown in Fig. 2(e), is 2.5 $\mu_B$. As the temperature increases, $M$ decreases. At room temperature (300 K), the Stoner and spin-fluctuation models predict 1.9 and 1.5 $\mu_B$ respectively for $M$. The Fe impurity still has a strong magnetic moment at room temperature because of the high $T_C$. This is very important for MoS$_2$ applications in spintronics and magnetic data storage.

![Image](image-url)

**Fig. 3** (a) Top view of the geometric structure of relaxed 10-ZMoS$_2$NR and its ten substitutional sites. (b) SPDOS of 10-ZMoS$_2$NR. (c) Top and (d) side views of the 0.02 eÅ$^3$ isosurface of the magnetization density distribution of the 10-ZMoS$_2$NR. Configuration-dependent (e) formation energy and (f) $M$ of 3d TM impurities of doped 10-ZMoS$_2$NRs.

The electronic and magnetic properties of zigzag MoS$_2$ nanoribbons (ZMoS$_2$NRs) doped with 3d TMs were also...
investigated. The relaxed structure of clean 10-ZMoS₂NR is shown in Fig. 3(a). From the SPDOS (Fig. 3(b)), 10-ZMoS₂NR shows spontaneous magnetization. The Mo 4d shows strong spin-polarization whereas the S 3sp is weakly spin-polarized. The 5 band gap of both majority and minority bands is zero. Thus 10-ZMoS₂NR is a metallic magnet. Each outermost Mo has the strongest magnetization, with a local magnetic moment of 0.7 μB whereas each outermost S has a local magnetic moment of 0.3 μB. The magnetization is mainly localized on the edges of 10-ZMoS₂NR (see Fig. 3(c) and (d)).

3d TM impurities are used to dope the 10-ZMoS₂NR to modulate the electronic and magnetic properties. Ten substitutional sites of 3d TM dopant with a concentration of 2.5 percent are considered for the 10-ZMoS₂NR (Fig. 3(a)). The width of the relaxed 10-ZMoS₂NR is around 2.6 nm. The stabilities of the configurations are analyzed by comparing the formation energies of different configurations (see Fig. 3(e)). For Mn-, Fe-, and Co-doped 10-ZMoS₂NRs, configuration 10 has the lowest formation energy because the bonds between the impurities and host atoms can be fully relaxed at the edges. Configuration 1 has the second lowest formation energy. Configuration 6 has the largest formation energy because the relaxation of the bonds between impurities and host atoms are restricted. This can be interpreted as an edge effect in which the formation energy is lower the nearer the impurities are to the edge. This is in agreement with experimental scanning transmission electron microscopy (STEM) findings that Co impurities replace the cations at the Mo edges of MoS₂ nanowires. Although there is rarely experimental reports on the 30 substitutional behaviors of Mn and Fe of Mo in MoS₂, from a thermodynamic point of view, we predict that Mn and Fe will also replace the cations at the Mo edges of MoS₂.

From Fig. 3(f), the 3d TM impurities of configuration 10 have the largest magnetic moment with Mn, Fe, and Co having local magnetic moments of 3.3, 2.4, and 1.0 μB respectively. Similarly, Mn, Fe, and Co adatoms on the MoS₂ monolayer have local magnetic moments of 3.0, 2.0, and 1.0 μB respectively. Impurities of the 3d TM-doped 10-ZMoS₂NRs exhibit obvious configuration-dependent magnetic properties. The nearer the impurities are to the edge, the larger the magnetic moments are.

To investigate the magnetic exchange coupling between impurities, we increased the dopant concentration to 5 percent. For the calculated structures of 10-ZMoS₂NR doped with Co-impurity pairs (Fig. 4(a) and (b)), the total energy of configuration γ is 0.16 eV smaller than that of configuration δ; thus configuration γ is more stable than configuration δ. Co impurities are distributed uniformly at the Mo edge. For Mn- and Fe-doped 10-ZMoS₂NRs, the total energy of configuration γ is 0.11 and 0.03 eV respectively smaller than that of configuration δ, and hence Mn and Fe are also distributed uniformly at the Mo edge. For Co-doped 10-ZMoS₂NRs with configuration γ, there is strong structural reconstruction at the Mo edge (Fig. 4(a)). Co atoms are relaxed towards interior sites of 10-ZMoS₂NR and form bonds with neighboring Mo atoms, and thereby stabilize this configuration γ. From experimental STEM images, configuration γ appears for Co-doped WS₂ nanowires.

### Table 2: Summary of ∆E (meV) for 3d TM impurity-doped ZMoS₂NRs with different widths. γ and δ indicate the configurations γ and δ, respectively.

<table>
<thead>
<tr>
<th></th>
<th>6_γ</th>
<th>6_δ</th>
<th>8_γ</th>
<th>8_δ</th>
<th>10_γ</th>
<th>10_δ</th>
<th>12_γ</th>
<th>12_δ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mn</td>
<td>76</td>
<td>-86</td>
<td>103</td>
<td>-88</td>
<td>115</td>
<td>-79</td>
<td>107</td>
<td>-83</td>
</tr>
<tr>
<td>Fe</td>
<td>30</td>
<td>28</td>
<td>32</td>
<td>35</td>
<td>26</td>
<td>48</td>
<td>23</td>
<td>51</td>
</tr>
<tr>
<td>Co</td>
<td>74</td>
<td>66</td>
<td>78</td>
<td>70</td>
<td>69</td>
<td>71</td>
<td>73</td>
<td>75</td>
</tr>
</tbody>
</table>

Fig. 4 Top views of Fe-impurity-pair-doped 10-ZMoS₂NRs with configuration (a) γ and (b) δ. (c) 0.02 e/Å³ isosurface and (d) SPDOS of the FM state of configuration γ. (e) Temperature-dependent M of Co impurity in doped 10-ZMoS₂NR with configuration γ.
From Table 2, \( \Delta E \) is 68 and 71 meV for the configurations \( \gamma \) and \( \delta \), respectively, of Co-doped 10-ZMoS\(_2\)NRs. Each Co impurity has a magnetic moment of 1.0 \( \mu_B \), thus we can take \( S=S_f=S_s=0.5 \) here. According to \( J=\Delta E/(4S_fS_s) \), the magnetic exchange coupling is 69 and 71 meV for configurations \( \gamma \) and \( \delta \), respectively. The corresponding \( T_C \) is 398 and 410 K calculated by eqn (4). Thus Co-doped 10-ZMoS\(_2\)NR manifests a strong FM nature with \( T_C \) above room temperature. The magnetization distribution of Co-doped 10-ZMoS\(_2\)NRs with configuration \( \gamma \). Fig. 4(c) shows the magnetization is mainly distributed on the edgiest S and Co atoms. Each edgiest S has a local magnetic moment of 0.4 \( \mu_B \), which is 0.1 \( \mu_B \) larger than that of clean 10-ZMoS\(_2\)NR. Thus doping the right Mo edge with Co impurities could also influence the magnetic properties of the left S edge of 10-ZMoS\(_2\)NR. These two edges contribute mainly to the states near the Fermi level and dominate the physical properties of 10-ZMoS\(_2\)NR. 

The DOS of the FM state for Co-doped 10-ZMoS\(_2\)NR with configuration \( \gamma \) (Fig. 4(d)) shows the Co impurities exhibit strong spin-polarization. For both spin-up and spin-down bands, the electrons occupy the Fermi-level states. Co-doped 10-ZMoS\(_2\)NR is still metallic, but the DOS distribution near the Fermi level has been strongly tuned by impurities in contrast to clean 10-ZMoS\(_2\)NR. The temperature-dependent magnetic moment of Co-doped 10-ZMoS\(_2\)NR (Fig. 4(e)) shows that as the temperature increases, the magnetic moment decreases. At room temperature, the magnetic moment of the Co-impurity is 0.5 and 0.7 \( \mu_B \), predicted by spin-fluctuation and Stoner models, respectively.

From Table 2, \( \Delta E \) is positive for Co-doped 6-, 8-, and 12-ZMoS\(_2\)NRs, so these ZMoS\(_2\)NRs also possess an FM ground state. According to eqn (4), the \( T_C \)s of these Co-doped ZMoS\(_2\)NRs are also above room temperature. 

Also from Table 2, Mn-doped ZMoS\(_2\)NRs exhibit configuration-dependent magnetic properties. Configuration \( \gamma \) is FM, whereas configuration \( \delta \) is AFM. For Mn-doped 10-ZMoS\(_2\)NR, we can take \( S=S_f=S_s=1.65 \), because each Mn has a local magnetic moment of 3.3 \( \mu_B \). In accordance with \( J=\Delta E/(4S_fS_s) \), the magnetic exchange coupling is 10.9 and 7.3 meV for configurations \( \gamma \) and \( \delta \), respectively. The \( T_C \) is 355 K for configuration \( \gamma \) calculated by eqn (4). For Mn-doped ZMoS\(_2\)NRs, configuration \( \delta \) exhibits AFM characteristics due to the superexchange interaction between the nearest-neighbor Mn atoms, while in configuration \( \gamma \) the impurities are remote. Similar effects were also found for Mn doped ZnO with impurities in the nearest-neighbor configuration.\(^{28,29}\)

All Fe-doped ZMoS\(_2\)NRs exhibit FM characteristics. Regarding Fe-doped 10-ZMoS\(_2\)NRs, we can take \( S=S_f=S_s=1.2 \) here as each Fe has a local magnetic moment of 2.4 \( \mu_B \). From \( J=\Delta E/(4S_fS_s) \), the magnetic exchange coupling is 4.5 and 8.3 meV for configurations \( \gamma \) and \( \delta \), respectively, with corresponding \( T_C \) of 91 and 169 K. Again, the \( T_C \)s are well below room temperature, thus Fe-doped 10-ZMoS\(_2\)NRs manifest weak FM characteristics. Although ZMoS\(_2\)NRs are natural magnetic, incorporating 3d TM impurities could further tune their magnetic and electronic properties.

**Conclusions**

In summary, the electronic and magnetic properties of MoS\(_2\) nanoribbons can be tuned with 3d TM impurities. These impurities tend to substitute the edgiest cations of AMoS\(_2\)NRs and ZMoS\(_2\)NRs. Fe-doped AMoS\(_2\)NRs manifest a FM semiconductor nature and their \( T_C \) can be tuned by adding impurities. In contrast, Co and Mn-doped AMoS\(_2\)NRs are AFM semiconductors. Co-doped ZMoS\(_2\)NRs show metallic and strong FM characteristics with \( T_C \) above room temperature. Mn-doped ZMoS\(_2\)NRs show configuration-dependent magnetic properties. Fe-doped ZMoS\(_2\)NRs are weak FM semiconductors. Our results provide an insight at the atomic level of the electronic and magnetic properties of 3d TM-doped MoS\(_2\) nanoribbons and pave the way for future applications of MoS\(_2\) and other transition metal dichalcogenides in nanoelectronic and spintronic devices.

**Acknowledgements**

The author gratefully acknowledges financial support from National Natural Science Foundation of China (Nos. 11304206 and 21001051), National Natural Science Foundation of Shenzhen University (Nos. 827000001 and 8270002601) and Strategic Emerging Industry Development Special Fund of Shenzhen (JCYJ20130326111743703 and JC201105170651A) and Shenzhen Key Laboratory of Sensor Technology Open Project (SST201302) and Shenzhen Key Laboratory of Special Functional Materials Open Project (T201302). The authors would thank the National Supercomputing Center in Shenzhen and the High Performance Computing Center of Shenzhen University for the computational facilities.
Notes and references

* College of Physics and Technology and Shenzhen Key Laboratory of Sensor Technology, Shenzhen University, Shenzhen 518060, Guangdong, P. R. China. E-mail: dayu@szu.edu.cn
5 b) Department of Mechanical Engineering and Materials Science, Department of Chemistry, and the Smalley Institute for Nanoscale Science and Technology, Rice University, Houston, Texas 77005, United States. E-mail: biy@rice.edu

Department of Electronic Engineering and Materials Science and Technology Research Center, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong SAR, People’s Republic of China


