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# Doping finite-length carbon and boron nitride nanotubes with aluminium atom: A thermodynamic semiempirical investigation

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## ABSTRACT

The doping reaction of truncated boron nitride and carbon nanotubes with aluminium atom was theoretically investigated. The AM1, PM3, and PM6 semiempirical methods have been used to evaluate the thermochemistry of doping reactions of single walled boron nitride nanotubes and carbon nanotubes. The enthalpy changes, Gibbs free energy changes, and entropy changes of studied doping reactions were evaluated at different temperatures. The AM1 and PM6 results showed Al-doping reaction of (8,0)CNT is exothermic and spontaneous . Among the studied armchair and zigzag nanotubes, AM1 and PM6 calculations reveal that (8,0)CNT is the best candidate for Al-doping reaction.

**Keywords:** Semiempirical methods; Doped nanotubes; Thermodynamic functions

## INTRODUCTION

Doping of boron nitride nanotubes (BNNTs) and carbon nanotubes (CNTs) is an effective way to extensively modify their various properties [1-4]. The doped nanotubes can exhibit dramatic changes with respect to the undoped-material [5]. For example, while C-doped BNNTs reduce the electronic band gaps, BNNTs are mainly insulator [6]. Doping of carbon nanotubes with boron (B) and nitrogen (N) are also possible which can engineer the electronic band-gap of CNTs [7]. The doped nanotubes are also investigated for their potential applications as adsorbents [5,8-10]. Methods based on the semiempirical potentials and, in particular the AM1 [11], allow to describe correctly the electronic structure and the reactivity of CNTs [12-15]. Wang et al. evaluated boundary orbitals, HOMO, and LUMO energies of single walled nanotubes (SWNTs) in a number of benzenoids along the peripheral circuit of the tubes by semiempirical PM3 method [16]. Mercuri employed AM1 semiempirical method to study of various electronic structures of finite-length models of CNTs on the basis of Clar sextet theory [17]. In the study of

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scavenging characteristic of SWNTs for OH radicals, the semiempirical PM6 method was used for geometry optimization of carbon nanotubes [18].

In this study, we performed a systematic semiempirical calculations to investigate the thermochemical aspects of doping single walled BNNTs and CNTs (armchair and zigzag 4,4and 8,0 CNTs and BNNTs) with aluminium atom (Fig.1).

## COMPUTIONAL METHODS

First, we constructed the (8,0) zigzag and the (4,4) armchair CNT and BNNTs and optimized them using semiempirical methods. Then, we doped each of them with one atom of aluminium and calculations were allowed to be continued.

All nanotube lengths were about 1nm, open-ended and defect free. The two caps of all nanotubes were saturated with hydrogen atoms to simulate the effect of a longer nanotube and also to prevent dangling of the nanotube terminal bonds. Moreover, the hydrogen atoms decrease the cost of the calculation as well [19]. As Fig. 1 reveals, the doping process is accompanied by replacing one carbon atom of nanotube by one aluminium atom. In the BNNTs there are two atoms (B atom and N atom) which can be replaced with one Al atom.

When boron atom is replaced with aluminum atom we named it as Al (*B*)-doped (4, 4) BNNT, and for replacement of nitrogen atom with Al atom we named the resulted structure as Al(*N*)-doped (4, 4) BNNT. When nitrogen atom of (4,4)BNNT is replaced with Al atom, a rough disarrangement was created in the structure of (4,4)BNNT. Due to this disarrangement, we did not consider the Al(*N*)-doped(4,4)BNNT for doping process.

The semiempirical methods, AM1 [20], PM3 [21], and PM6 [22] were used to optimize the studied models. These methods are implemented in the MOPAC program package [23]. Furthermore, frequency calculations were carried out to confirm the stability of considered structures and to obtain thermochemical functions. The frequency calculations were performed at 1 atm and temperature was allowed to increase by step of 5 degrees of Kelvin starting from 298.15 K. In order to evaluate the thermodynamic functions of the doping reactions we used the following model:

$$\mathrm{SWNT} + \mathrm{Al} = \mathrm{Al-doped\ SWNT} + \mathrm{C} \qquad (1)$$

where, C denotes carbon atom.

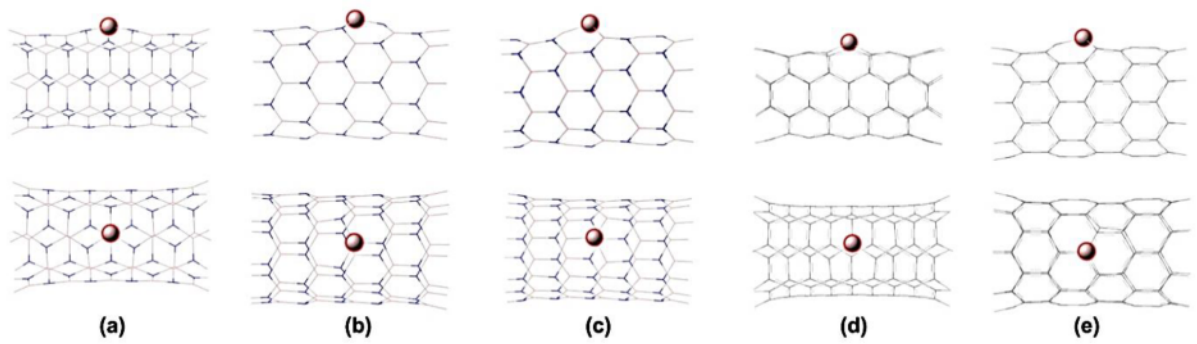


**Fig.1.** The optimized structures of (a) Al(*B*)-doped (4,4)BNNT (b) Al(*B*)-doped (8,0)BNNT (c) Al(*N*)-doped (8,0)BNNT (d) Al-doped (4,4)CNT (e) Al-doped (8,0)CNT.

# RESULTS AND DISCUSSIONS

## AM1 method

For Al(B)-doped(4,4)BNNT, in all considered temperatures, the doping reaction is endothermic and nonspontaneous (Table 1). For Al(B)-doped(8,0)BNNT, the doping reaction is also endothermic and nonspontaneous (Table 1). The Al doping reaction is more endothermic for (4, 4)BNNT than the (8,0)BNNT. Moreover, the Al-doping for (8,0)BNNT is harder to perform than the (4,4)BNNT due to more positive values of $\Delta_rG_{doping}$. The Al(N)-doped(8,0)BNNT formation is even more endothermic and nonspontaneous. There was negative $\Delta_rS_{doping}$ for Al(B)-doped(8,0)BNNT while $\Delta_rS_{doping}$ was positive for all other nanotubes (Table 1). The doping reaction of (4,4)CNT like BNNTs was endothermic and nonspontaneous while (8,0)CNT doping reaction was exothermic and spontaneous (Table 1). The AM1 results support zigzag (8,0)CNT as potential candidate for doping by Al atom.

## PM3 method

Based on the results of PM3 method, the doping reactions for none of the studied nanotubes were favorable (Table 2). All Al-doping reactions present positive $\Delta_rH_{doping}$ and $\Delta_rG_{doping}$ values indicating that all considered nanotubes are not suitable for doping with aluminium atom. Enthalpy increasing with temperature for all doping reactions was not significant. On the other hand, by temperature increment, the $\Delta_rG_{doping}$ of BNNTs increases while for CNTs doping the $\Delta_rG_{doping}$ decreasing (Table 2). The PM3 method results negative $\Delta_rS_{doping}$for Al(B)-doped(4,4)BNNT and Al(B)-doped(8,0)BNNT while for the rest of nanotubes, corresponding values are positive. As Table 2 shows, increasing of $\Delta_rS_{doping}$ with temperature for CNTs is sharper than the BNNTs.

## PM6 method

According to the enthalpy and Gibbs free energy changes provided at the AM1 (Table 1) and PM3 (Table 2) levels, a same trend can be pointed out for $\Delta_rH_{doping}$ and $\Delta_rG_{doping}$; that is, $\Delta_rH_{doping}$ and $\Delta_rG_{doping}$ for BNNTs and (4,4)CNT doping are positive (endothermic and nonspontaneous). However, the entropy changes present different trend. The $\Delta_rS_{doping}$ at the PM6 level is negative for Al(B)-doped(4,4)BNNT and Al(B)-doped(8,0)BNNT, and positive for Al-doped(4,4)CNT and Al-doped(8,0)CNT in all studied temperatures. Here like the AM1 method, the Al-doping reaction of (8,0)CNT is exothermic and spontaneous.

# CONCLUSIONS

We theoretically investigated the finite-length armchair and zigzag boron nitride, and carbon nanotubes for doping with Al atom. All nanotubes were single-walled and finite length with hydrogen saturation in the terminal atoms. The semi-empirical quantum chemistry techniques AM1, PM3, and PM6 were used for the study. The results of AM1, PM3, and PM6 showed the same trends for enthalpy and Gibbs free energy changes for Al-doping reactions of BNNTs and (4,4)CNT. The thermodynamic calculations based on the semiempirical AM1 and PM6 levels results showed that the zigzag (8,0)CNT is the best candidate for doping with aluminum atom at different studied temperature.

**Table 1.** Calculated thermodynamic functions ($\Delta H$ kJ/mol, $\Delta G$ kJ/mol, and $\Delta S$ kJ/mol.K) of doping reactions at AM1 semiempirical level of theory

| Temperature (K) | Thermo- function | Doping reaction product | | | | |
|---|---|---|---|---|---|---|
| | | Al($B$)-doped (8,0)BNNT | Al($B$)-doped (8,0)BNNT | Al($N$)-doped (8,0)BNNT | Al-doped (4,4)CNT | Al-doped (8,0)CNT |
| **298.15** | $\Delta_r H_{doping}$ | 750.65 | 762.68 | 1126.83 | 183.47 | -70.36 |
| | $\Delta_r G_{doping}$ | 456.98 | 764.08 | 1125.79 | 172.77 | -85.51 |
| | $\Delta_r S_{doping}$ | 0.9850 | -0.0047 | 0.0035 | 0.0359 | 0.0508 |
| **303.15** | $\Delta_r H_{doping}$ | 750.70 | 762.73 | 1126.92 | 183.70 | -70.09 |
| | $\Delta_r G_{doping}$ | 448.27 | 764.10 | 1125.77 | 172.59 | -85.77 |
| | $\Delta_r S_{doping}$ | 0.9976 | -0.0045 | 0.0038 | 0.0367 | 0.0517 |
| **308.15** | $\Delta_r H_{doping}$ | 750.75 | 762.78 | 1127.00 | 183.94 | -69.81 |
| | $\Delta_r G_{doping}$ | 439.42 | 764.12 | 1125.75 | 172.41 | -86.03 |
| | $\Delta_r S_{doping}$ | 1.01 | -0.0044 | 0.0041 | 0.0374 | 0.0526 |
| **313.15** | $\Delta_r H_{doping}$ | 750.80 | 762.83 | 1127.09 | 184.17 | -69.53 |
| | $\Delta_r G_{doping}$ | 430.44 | 764.14 | 1125.72 | 172.21 | -86.30 |
| | $\Delta_r S_{doping}$ | 1.02 | -0.0042 | 0.0044 | 0.0382 | 0.0535 |
| **318.15** | $\Delta_r H_{doping}$ | 750.85 | 762.88 | 1127.18 | 184.41 | -69.26 |
| | $\Delta_r G_{doping}$ | 421.33 | 764.16 | 1125.71 | 172.02 | -86.57 |
| | $\Delta_r S_{doping}$ | 1.04 | -0.0040 | 0.0046 | 0.0390 | 0.0544 |
| **323.15** | $\Delta_r H_{doping}$ | 750.90 | 762.93 | 1127.26 | 184.65 | -68.98 |
| | $\Delta_r G_{doping}$ | 412.09 | 764.19 | 1125.68 | 171.83 | -86.84 |
| | $\Delta_r S_{doping}$ | 1.05 | -0.0039 | 0.0049 | 0.0397 | 0.0553 |
| **328.15** | $\Delta_r H_{doping}$ | 750.95 | 765.70 | 1130.07 | 184.89 | -68.70 |
| | $\Delta_r G_{doping}$ | 402.72 | 764.20 | 1125.66 | 171.62 | -87.12 |
| | $\Delta_r S_{doping}$ | 1.06 | 0.0046 | 0.0135 | 0.0404 | 0.0561 |
| **333.15** | $\Delta_r H_{doping}$ | 751.00 | 763.02 | 1127.43 | 185.13 | -68.43 |
| | $\Delta_r G_{doping}$ | 393.22 | 764.22 | 1125.63 | 171.42 | -87.40 |
| | $\Delta_r S_{doping}$ | 1.07 | -0.0036 | 0.0054 | 0.0412 | 0.0569 |
| **338.15** | $\Delta_r H_{doping}$ | 751.04 | 763.07 | 1127.51 | 185.37 | -68.16 |
| | $\Delta_r G_{doping}$ | 383.59 | 764.24 | 1125.60 | 171.21 | -87.69 |
| | $\Delta_r S_{doping}$ | 1.09 | -0.0035 | 0.0056 | 0.0419 | 0.0578 |
| **343.15** | $\Delta_r H_{doping}$ | 751.10 | 763.12 | 1127.60 | 185.62 | -67.88 |
| | $\Delta_r G_{doping}$ | 373.83 | 764.26 | 1125.57 | 171.00 | -87.98 |
| | $\Delta_r S_{doping}$ | 1.10 | -0.0033 | 0.0059 | 0.0426 | 0.0586 |
| **348.15** | $\Delta_r H_{doping}$ | 751.14 | 763.17 | 1127.68 | 185.86 | -67.60 |
| | $\Delta_r G_{doping}$ | 363.94 | 764.27 | 1125.54 | 170.79 | -88.27 |
| | $\Delta_r S_{doping}$ | 1.11 | -0.0032 | 0.0062 | 0.0433 | 0.0594 |

**Table 2.** Calculated thermodynamic functions ($\Delta H$ kJ/mol, $\Delta G$ kJ/mol, and $\Delta S$ kJ/mol.K) of doping reactions at PM3 semiempirical level of theory

| Temperature (K) | Thermo-function | Doping reaction product | | | | |
|---|---|---|---|---|---|---|
| | | Al($B$)-doped (4,0)BNNT | Al($B$)-doped (8,0)BNNT | Al($N$)-doped (8,0)BNNT | Al-doped (4,4)CNT | Al-doped (8,0)CNT |
| **298.15** | $\Delta_r H_{doping}$ | 869.760 | 874.27 | 1199.52 | 455.77 | 31.16 |
| | $\Delta_r G_{doping}$ | 873.46 | 874.87 | 1198.17 | 443.78 | 14.20 |
| | $\Delta_r S_{doping}$ | -0.01242 | -0.00202 | 0.0045 | 0.0402 | 0.0569 |
| **303.15** | $\Delta_r H_{doping}$ | 869.766 | 874.31 | 1199.57 | 456.02 | 31.46 |
| | $\Delta_r G_{doping}$ | 873.53 | 874.88 | 1198.14 | 443.57 | 13.92 |
| | $\Delta_r S_{doping}$ | -0.01241 | -0.00189 | 0.0047 | 0.0411 | 0.0579 |
| **308.15** | $\Delta_r H_{doping}$ | 869.773 | 874.34 | 1199.63 | 456.27 | 31.76 |
| | $\Delta_r G_{doping}$ | 873.59 | 874.89 | 1198.12 | 443.36 | 13.62 |
| | $\Delta_r S_{doping}$ | -0.01238 | -0.00178 | 0.0049 | 0.0419 | 0.0589 |
| **313.15** | $\Delta_r H_{doping}$ | 869.776 | 874.38 | 1199.68 | 456.53 | 32.06 |
| | $\Delta_r G_{doping}$ | 873.66 | 874.90 | 1198.10 | 443.15 | 13.33 |
| | $\Delta_r S_{doping}$ | -0.01239 | -0.00168 | 0.0051 | 0.0427 | 0.0598 |
| **318.15** | $\Delta_r H_{doping}$ | 869.784 | 874.41 | 1199.73 | 456.78 | 32.36 |
| | $\Delta_r G_{doping}$ | 873.72 | 874.91 | 1198.07 | 442.94 | 13.02 |
| | $\Delta_r S_{doping}$ | -0.01237 | -0.00155 | 0.0052 | 0.0435 | 0.0608 |
| **323.15** | $\Delta_r H_{doping}$ | 869.787 | 874.44 | 1199.79 | 457.03 | 32.66 |
| | $\Delta_r G_{doping}$ | 873.78 | 874.91 | 1198.04 | 442.71 | 12.72 |
| | $\Delta_r S_{doping}$ | -0.01237 | -0.00145 | 0.0054 | 0.0443 | 0.0617 |
| **328.15** | $\Delta_r H_{doping}$ | 869.794 | 874.48 | 1199.84 | 457.29 | 32.97 |
| | $\Delta_r G_{doping}$ | 873.85 | 874.92 | 1198.02 | 442.49 | 12.41 |
| | $\Delta_r S_{doping}$ | -0.01237 | -0.00135 | 0.0056 | 0.0451 | 0.0626 |
| **333.15** | $\Delta_r H_{doping}$ | 869.800 | 874.51 | 1199.89 | 457.55 | 33.26 |
| | $\Delta_r G_{doping}$ | 873.92 | 874.93 | 1197.99 | 442.27 | 12.10 |
| | $\Delta_r S_{doping}$ | -0.01236 | -0.00125 | 0.0057 | 0.0459 | 0.0635 |
| **338.15** | $\Delta_r H_{doping}$ | 869.805 | 874.55 | 1199.94 | 457.80 | 33.56 |
| | $\Delta_r G_{doping}$ | 873.98 | 874.94 | 1197.96 | 442.04 | 11.78 |
| | $\Delta_r S_{doping}$ | -0.01235 | -0.00116 | 0.0059 | 0.0466 | 0.0644 |
| **343.15** | $\Delta_r H_{doping}$ | 869.810 | 874.58 | 1199.99 | 458.06 | 33.87 |
| | $\Delta_r G_{doping}$ | 874.04 | 874.94 | 1197.93 | 441.80 | 11.45 |
| | $\Delta_r S_{doping}$ | -0.01232 | -0.00105 | 0.0060 | 0.0474 | 0.0653 |
| **348.15** | $\Delta_r H_{doping}$ | 869.815 | 874.61 | 1200.04 | 458.32 | 34.16 |
| | $\Delta_r G_{doping}$ | 874.10 | 874.94 | 1197.89 | 441.56 | 11.12 |
| | $\Delta_r S_{doping}$ | -0.01232 | -0.00095 | 0.0062 | 0.0481 | 0.0662 |

**Table 3.** Calculated thermodynamic functions ($\Delta H$ kJ/mol, $\Delta G$ kJ/mol, and $\Delta S$ kJ/mol.K) of doping reactions at PM6 semiempirical level of theory

| Temperature (K) | Thermo-function | Doping reaction product | | | | |
|---|---|---|---|---|---|---|
| | | Al(*B*)-doped (4,0)BNNT | Al(*B*)-doped (8,0)BNNT | Al(*N*)-doped (8,0)BNNT | Al-doped (4,4)CNT | Al-doped (8,0)CNT |
| **298.15** | $\Delta_r H_{doping}$ | 749.09 | 761.90 | 986.57 | 442.15 | -169.66 |
| | $\Delta_r G_{doping}$ | 749.82 | 762.95 | 986.648 | 433.74 | -183.68 |
| | $\Delta_r S_{doping}$ | -0.0025 | -0.0035 | -0.00026 | 0.0282 | 0.047 |
| **303.15** | $\Delta_r H_{doping}$ | 749.14 | 761.94 | 986.62 | 442.33 | -169.41 |
| | $\Delta_r G_{doping}$ | 749.84 | 762.97 | 986.651 | 433.61 | -183.91 |
| | $\Delta_r S_{doping}$ | -0.0023 | -0.0034 | -0.0001 | 0.0288 | 0.0478 |
| **308.15** | $\Delta_r H_{doping}$ | 749.19 | 761.99 | 986.68 | 442.51 | -169.16 |
| | $\Delta_r G_{doping}$ | 749.85 | 762.98 | 986.653 | 433.47 | -184.16 |
| | $\Delta_r S_{doping}$ | -0.0021 | -0.0032 | 0.00009 | 0.0293 | 0.0487 |
| **313.15** | $\Delta_r H_{doping}$ | 749.24 | 762.03 | 986.73 | 442.68 | -168.92 |
| | $\Delta_r G_{doping}$ | 749.86 | 763.00 | 986.651 | 433.32 | -184.4 |
| | $\Delta_r S_{doping}$ | -0.0020 | -0.0031 | 0.00026 | 0.0299 | 0.0494 |
| **318.15** | $\Delta_r H_{doping}$ | 749.29 | 762.08 | 986.79 | 442.86 | -168.67 |
| | $\Delta_r G_{doping}$ | 749.87 | 763.01 | 986.648 | 433.17 | -184.65 |
| | $\Delta_r S_{doping}$ | -0.0018 | -0.0029 | 0.00045 | 0.0304 | 0.0502 |
| **323.15** | $\Delta_r H_{doping}$ | 749.33 | 762.12 | 986.84 | 443.03 | -168.42 |
| | $\Delta_r G_{doping}$ | 749.88 | 763.03 | 986.645 | 433.01 | -184.90 |
| | $\Delta_r S_{doping}$ | -0.0017 | -0.0028 | 0.0006 | 0.031 | 0.051 |
| **328.15** | $\Delta_r H_{doping}$ | 749.38 | 762.16 | 986.89 | 443.20 | -168.17 |
| | $\Delta_r G_{doping}$ | 749.89 | 763.04 | 986.643 | 432.85 | -185.16 |
| | $\Delta_r S_{doping}$ | -0.0015 | -0.0027 | 0.00077 | 0.0316 | 0.0518 |
| **333.15** | $\Delta_r H_{doping}$ | 749.43 | 762.21 | 986.95 | 443.38 | -167.91 |
| | $\Delta_r G_{doping}$ | 749.89 | 763.05 | 986.64 | 432.69 | -185.42 |
| | $\Delta_r S_{doping}$ | -0.0014 | -0.0025 | 0.00094 | 0.0321 | 0.0526 |
| **338.15** | $\Delta_r H_{doping}$ | 749.48 | 762.25 | 987.00 | 443.56 | -167.66 |
| | $\Delta_r G_{doping}$ | 749.90 | 763.06 | 986.632 | 432.53 | -185.69 |
| | $\Delta_r S_{doping}$ | -0.0013 | -0.0024 | 0.00109 | 0.0326 | 0.0533 |
| **343.15** | $\Delta_r H_{doping}$ | 749.53 | 762.30 | 987.06 | 443.75 | -167.41 |
| | $\Delta_r G_{doping}$ | 749.91 | 763.08 | 986.627 | 432.36 | -185.95 |
| | $\Delta_r S_{doping}$ | -0.0011 | -0.0023 | 0.00125 | 0.0332 | 0.054 |
| **348.15** | $\Delta_r H_{doping}$ | 749.57 | 762.34 | 987.11 | 443.92 | -167.15 |
| | $\Delta_r G_{doping}$ | 749.91 | 763.09 | 986.619 | 432.20 | -186.23 |
| | $\Delta_r S_{doping}$ | -0.0010 | -0.0021 | 0.00141 | 0.0337 | 0.0548 |

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