# INTISARI

## PEMODELAN *DOPING* NITROGEN DALAM *CARBON NANOTUBE* (6,0) DENGAN TEORI FUNGSI KERAPATAN

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*Doping* nitrogen dalam *Carbon Nanotube* (CNT) merupakan salah satu cara untuk memodifikasi struktur CNT agar memiliki sifat elektronik sesuai dengan kebutuhan. Pemodelan *doping* nitrogen dalam CNT dengan kiralitas (6,0) bertujuan untuk memberikan informasi teoritik tentang pengaruh *doping* nitrogen terhadap struktur dan sifat elektronik CNT. Informasi tersebut diperlukan untuk memprediksi arah dan kondisi eksperimen dalam sintesis CNT ter-*doping* nitrogen.

Pemodelan dilakukan dengan metode Teori Fungsi Kerapatan/ *Density Functional Theory* (DFT) pada tingkatan teori hibrid Becke 3, Lee-Yang-Parr (B3LYP). Pemodelan dilakukan melalui substitusi atom karbon dengan atom nitrogen membentuk struktur *graphite-like* dan *pyridine-like*. Substitusi atom karbon dengan atom nitrogen dilakukan secara acak. Konsentrasi dopan nitrogen dalam CNT yang membentuk struktur *graphite-like* adalah 2,37% dan 4,73% sedangkan untuk *pyridine-like* adalah 2,42% dan 4,83%. Pengaruh *doping* nitrogen terhadap struktur dan sifat elektronik CNT dimodelkan melalui perhitungan parameter struktur (diameter, panjang ikatan, energi kohesif dan momen dipol) serta parameter sifat elektronik (*Density of State* (DOS), celah energi antara energi HOMO (*Highest Occupied Molecular Orbital*) dan LUMO (*Lowest Unoccupied Molecular Orbital*), potensial ionisasi, afinitas elektron, *hardness*, energi vibrasi ikatan dan energi eksitasi elektron) CNT (6,0) murni maupun ter-*doping* nitrogen.

Hasil penelitian menunjukkan bahwa celah energi antara HOMO dan LUMO pada CNT dipengaruhi oleh panjang tabung, diameter dan kiralitas CNT. *Doping* nitrogen dalam CNT menyebabkan peningkatan diameter (dari 4,82 Å menjadi 4,83 – 4,85 Å), momen dipol (dari 0,0 Debye menjadi 0,21 – 3,36 Debye), energi kohesif (dari 260,97 kkal/mol menjadi 1401,73 – 2580,98 kkal/mol), celah energi antara energi HOMO dan LUMO (dari 0,43 eV menjadi 0,64 – 1,88 eV), potensial ionisasi (dari 3,65 eV menjadi 3,82 – 4,71 eV), *hardness* (dari 0,21 eV menjadi 0,32 – 0,94 eV), energi vibrasi ikatan dan eksitasi elektron serta meningkatkan kestabilan CNT. *Doping* nitrogen dalam CNT menurunkan DOS pada daerah Fermi, energi Fermi, dan afinitas elektron. Variasi konsentrasi dopan nitrogen dalam CNT berpengaruh terhadap sifat elektronik CNT. Semakin tinggi konsentrasi dopan nitrogen dalam CNT semakin rendah kestabilan dan semakin kecil lebar celah antara energi HOMO dan LUMO.

**Kata kunci**: DFT, *Carbon Nanotube* (CNT), *doping*, sifat elektronik

# ABSTRACT

## THE MODELLING OF NITROGEN DOPING IN CARBON NANOTUBE (6,0) BY USING DENSITY FUNCTIONAL THEORY

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Nitrogen doping in Carbon Nanotube (CNT) is a way to modify the structure of CNT in order to produce CNT that has appropriate electronic property. The modelling of nitrogen doping in CNT with chirality (6,0) is aimed at giving theoretical information about the effect of nitrogen doping toward the structure and electronic property of CNT. That information is really needed to predict the direction and experiment condition in CNT synthesis with nitrogen doping.

The modelling was done by using Density Functional Theory (DFT) method at the level of hybrid theory Becke 3, Lee-Yang-Parr (B3LYP). The modelling was also done through atom carbon substitution with atom nitrogen that builds graphite-like and pyridine-like structure. The substitution of atom carbon with atom nitrogen was done randomly. The concentration of nitrogen dopan in CNT which build graphite-like structure is 2,37% and 4,73%, and for pyridine-like is 2,42% and 4,83%. The effect of nitrogen doping toward structure and electronic property of CNT was done by using the structure parameter measurement (diameter, bond length, cohesive energy, and dipole moment) and the parameter of electronic property (Density of State (DOS), gap width between HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) energy, ionization potential, electron affinity, hardness, bonding vibration energy, and electron excitation energy) CNT (6,0) in pure condition and with nitrogen doping.

The result of this research states that the energy gap between HOMO and LUMO at CNT is effected by the length, diameter and chirality of the tube. Nitrogen doping in CNT causes the diameter increase (from 4,82 Å becomes 4,83 – 4,85 Å), dipole moment (from 0,0 Debye becomes 0,21 – 3,36 Debye), cohesive energy (from 260,97 kkal/mol becomes 1401,73 – 2580,98 kkal/mol), the gap width between HOMO and LUMO energy (from 0,43 eV becomes 0,64 – 1,88 eV), ionization potential (from 3,65 eV becomes 3,82 – 4,71 eV), hardness (from 0,21 eV becomes 0,32 – 0,94 eV), bonding vibration energy and electron excitation, it also increases the CNT stability. Nitrogen doping in CNT decreases DOS at Fermi area (from 0,5 becomes 0,3 and 0), Fermi energy (from 3,43 eV becomes 3,50 – 3,81 eV), and electron affinity (from 3,22 eV becomes 3,18 – 2,58 eV). The variation of nitrogen dopan in CNT has an effect toward CNT electronic property. If the concentration becomes higher, the stability and gap energy becomes lower. The width of energy gap is 1,72 & 1,88 eV; 1,55 & 1,79 eV; 1,39 & 1,50 eV; and 0,64 eV gradually for dopan concentration 2,37%; 2,42%; 4,73 and 4,83%.

**Key words**: Carbon Nanotube (CNT), doping, density functional theory, electronic property