ABSTRAK

STUDI KOMPUTASI ADSORPSI GAS NO PADA *NANOCAGE* $X_{12}Y_{12}$ (X = B, In & Y = N, Sb) MENGGUNAKAN METODE *DENSITY FUNCTIONAL THEORY*

Peningkatan penggunaan bahan bakar minyak untuk kendaraan mengakibatkan peningkatan polusi udara seperti gas nitrogen monoksida (NO) yang sangat reaktif serta berbahaya bagi manusia dan lingkungan. Penggunaan sensor dari nanomaterial *nanocage* $X_{12}Y_{12}$ sangat potensial untuk mendeteksi polutan gas berbahaya, oleh karena itu penelitian ini membahas mengenai adsorpsi *nanocage* $X_{12}Y_{12}$ dengan tipe $B_{12}N_{12}$, $B_{12}Sb_{12}$, $In_{12}N_{12}$, dan $In_{12}Sb_{12}$ pada molekul gas NO yang dapat diaplikasikan sebagai sensor gas NO. Tujuan penelitian ini adalah menganalisis karakteristik, pengaruh interaksi dan kualitas adsorpsi antara molekul gas NO dengan *nanocage* $X_{12}Y_{12}$ dengan tipe $B_{12}N_{12}$, $B_{12}Sb_{12}$, $In_{12}N_{12}$, dan $In_{12}Sb_{12}$. Metode yang digunakan yaitu *Density Functional Theory* fungsional B3LYP dengan basis LANL2DZ serta koreksi dispersi D4. Hasilnya, adsorpsi NO pada *nanocage* terjadi melalui proses adsorpsi fisika. Nilai energi adsorpsi NO pada *nanocage* $B_{12}N_{12}$, $B_{12}Sb_{12}$, $In_{12}N_{12}$, dan $In_{12}Sb_{12}$ adalah -16,8032 kJ/mol, -4,4633 kJ/mol, -35,4442 kJ/mol, -17,8532 kJ/mol. Interaksi NO dengan *nanocage* $B_{12}N_{12}$ dan $In_{12}N_{12}$ adalah interaksi sedang dengan jenis ikatan kovalen parsial. Sedangkan, interaksi adsorpsi NO pada *nanocage* $B_{12}Sb_{12}$ dan $In_{12}Sb_{12}$ berjenis interaksi lemah. Interaksi antara molekul gas NO dengan *nanocage* mempengaruhi reaktivitas, stabilitas, transisi elektronik, dan jarak ikatan. Dengan demikian, dapat disimpulkan bahwa adsorpsi NO pada *nanocage* $In_{12}N_{12}$ merupakan adsorpsi paling baik dan potensial untuk diaplikasikan sebagai sensor gas NO.

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Kata-kata kunci: adsorpsi; DFT; *nanocage*; nanomaterial; nitrogen monoksida.

ABSTRACT

COMPUTATIONAL STUDY OF NO GAS ADSORPTION ON *NANOCAGE* $X_{12}Y_{12}$ (X = B, In & Y = N, Sb) USING DENSITY FUNCTIONAL THEORY METHODS

Increased use of fuel oil for vehicles results in increased air pollution, such as nitrogen monoxide (NO) gas, which is highly reactive and dangerous for humans and the environment. Using sensors from the $X_{12}Y_{12}$ nanocage nanomaterial has excellent potential for detecting dangerous gas pollutants. Therefore, this research discusses the adsorption of $X_{12}Y_{12}$ nanocage types $B_{12}N_{12}$, $B_{12}Sb_{12}$, $In_{12}N_{12}$, and $In_{12}Sb_{12}$ on NO gas molecules, which can be applied as a NO gas sensor. This research analyses the characteristics, interaction effects and adsorption quality between NO gas molecules and $X_{12}Y_{12}$ nanocages with types $B_{12}N_{12}$, $B_{12}Sb_{12}$, $In_{12}N_{12}$, and $In_{12}Sb_{12}$. The method used is Density Functional Theory B3LYP functional with LANL2DZ basis and D4 dispersion correction. As a result, NO adsorption on the nanocage occurred through a physical adsorption process. The NO adsorption energy values on $B_{12}N_{12}$, $B_{12}Sb_{12}$, $In_{12}N_{12}$, and $In_{12}Sb_{12}$ nanocages are -16.8032 kJ/mol, -4.4633 kJ/mol, -35.4442 kJ/mol, -17.8532 kJ/mol. The interaction of NO with $B_{12}N_{12}$ and $In_{12}N_{12}$ nanocages is a moderate interaction with a partial covalent bond type. Meanwhile, the NO adsorption interaction between $B_{12}Sb_{12}$ and $In_{12}Sb_{12}$ nanocages is weak. The interaction between NO gas molecules and nanocages affects reactivity, stability, electronic transitions,and bond distances. Thus, NO adsorption by the $In_{12}N_{12}$ nanocage is the best and has the potential to be applied as a NO gas sensor.

Keywords: Adsorption; DFT; nanocage; nanomaterial; nitrogen monoxide.

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