ABSTRAK

STUDI KOMPUTASI ADSORPSI GAS NO_2 OLEH *NANOCAGE* $X_{12}Y_{12}$ (X= B, In dan Y= N, Sb) MENGGUNAKAN METODE *DENSITY FUNCTIONAL THEORY* (DFT)

Peningkatan kadar polutan nitrogen dioksida dalam beberapa waktu terakhir dikaitkan dengan dampaknya terhadap kesehatan manusia dan dampak buruk terhadap lingkungan. Salah satu upaya untuk mengurangi jumlah NO_2 dilakukan dengan adsorpsi oleh nanomaterial berbasis *nanocage*. Pada penelitian ini dilakukan analisis untuk mengidentifikasi struktur, sifat elektronik, sifat fisik, dan pemahaman orbital molekul dari *nanocage*. Penelitian ini menggunakan perhitungan menggunakan metode *Density Functional Theory* (DFT) dengan level teori B3LYP, faktor dispersi D4, dan basis set LANLD2Z. Metode tersebut digunakan untuk energi celah HOMO-LUMO yang terhubung dengan parameter reaktivitas global, termasuk *chemical potential*, *ionization potential*, *chemical hardness*, dan *softness*. Selain itu, sifat elektronik *density of states (DOS), natural bond orbital (NBO), and electronical potential (ESP),* serta interaksi kimia dalam sistem seperti IGMH dan AIMD, juga disediakan. Hasil penelitian menunjukkan menunjukkan bahwa *nanocage* $X_{12}Y_{12}$ dapat mengadsorpsi gas NO_2 dalam berbagai jarak hingga 5000 fs. Reaksi *nanocage* $X_{12}Y_{12}$ dengan NO_2 bersifat spontan, eksoterm, dan bersifat kovalen parsial. Urutan *nanocage* yang paling efektif dalam menyerap gas NO_2 secara berturut-turut yaitu: $B_{12}Sb_{12} > B_{12}N_{12} < In_{12}N_{12} > In_{12}Sb_{12}$. $B_{12}Sb_{12}$ sangat sensitif terhadap molekul NO_2, dengan interaksi ikatan dan energi adsorpsi sebesar -307,93 kj/mol dan dibuktikan dengan grafik UV-vis dan IRI. Fenomena ini menunjukkan bahwa *nanocage* $B_{12}Sb_{12}$ memiliki potensi tinggi untuk menyerap gas NO_2.

Kata-kata kunci: adsorpsi; *density functional theory*; *nanocage*; nitrogen dioksida.

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SUNAN GUNUNG DJATI
BANDUNG

ABSTRACT

COMPUTATIONAL STUDY OF ADSORPTION OF NO_2 GAS BY NANOCAGE $X_{12}Y_{12}$ (X= B, In dan Y= N, Sb) USING DENSITY FUNCTIONAL THEORY (DFT) METHOD

Recent increases in nitrogen dioxide (NO_2) pollutant levels have been linked to adverse impacts on human health and the environment. One strategy to mitigate NO_2 concentrations involves adsorption using nanomaterial-based nanocages. This study investigates the structure, electronic properties, physical characteristics, and molecular orbital interactions of these nanocages. Density Functional Theory (DFT) calculations were performed using the B3LYP theoretical level, D4 dispersion corrections, and the LANL2DZ basis set. These methods were employed to determine the HOMO-LUMO gap energy, which correlates with global reactivity parameters such as chemical potential, ionization potential, chemical hardness, and softness. Additionally, electronic properties, including density of states (DOS), natural bond orbital (NBO) analysis, and electrostatic potential (ESP), as well as chemical interactions within the system such as IGMH and AIMD were analyzed. The results indicate that the $X_{12}Y_{12}$ nanocage can adsorb NO_2 gas at various distances up to 5000 femtoseconds. The interaction between the $X_{12}Y_{12}$ nanocage and NO_2 is spontaneous, exothermic, and partially covalent. The order of effectiveness for NO_2 gas adsorption among the nanocages is as follows: $B_{12}Sb_{12} > B_{12}N_{12} > In_{12}N_{12} > In_{12}Sb_{12}$. The $B_{12}Sb_{12}$ nanocage is particularly sensitive to NO_2 molecules, with a binding interaction and adsorption energy of -307.93 kJ/mol, as demonstrated by UV-Vis spectroscopy and the Independent Gradient Model-Hirshfeld (IGMH) analysis. These findings suggest that the $B_{12}Sb_{12}$ nanocage has significant potential for NO_2 gas adsorption.

Keywords: adsorption; density functional theory; nanocage; nitrogen dioxide.

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