KOMPUTASI PENGARUH PENAMBAHAN rGO PADA $LaFeO_3$ YANG DIDOPING Co TERHADAP ENERGI ADSORPSI MOLEKUL ETANOL MENGGUNAKAN *DENSITY FUNCTIONAL THEORY* UNTUK SENSOR GAS

SKRIPSI

Disusun untuk memenuhi sebagian dari syarat untuk memperoleh gelar Sarjana Sains Program Studi Fisika
Kelompok bidang kajian Fisika Material

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Sebuah skripsi yang diajukan untuk memenuhi salah satu syarat memperoleh gelar Sarjana Sains (S.Si) pada program Studi Fisika

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ABSTRAK

Material $LaFeO_3$ (LFO) telah banyak digunakan sebagai material penyusun sensor gas. Meskipun LFO sudah banyak diaplikasikan kedalam sensor gas, namun selektivitas dan sensitivitas serta temperatur kerja snesor gas masih belum optimal. LFO dalam penelitian ini diberikan doping Co dan juga dilapisi *single layer* rGO untuk menganalisis sensitivitas dan selektivitasnya berdasarkan energi adsorpsi dengan menggunakan *Density Functional Theory* (DFT). Berdasarkan penelitian ini, didapatkan bahwa dengan adanya doping Co dan lapisan rGO dapat meningkatkan energi adsorpsi pada LFO. Penambahan lapisan rGO pada LFO membuat peningkatan energi adsorpsi sebesar 23.58 % dari -2.38 eV untuk LFO doping Co menjadi -2.93 eV ketika ditambahkan rGO. Hal tersebut menunjukan potensi dari penambahan lapisan rGO pada material LFO untuk material sensor.

Kata kunci : $LaFeO_3$, Cobalt, sensor gas, gas etanol, *reduce graphene oxide, density functional theory,*

ABSTRACT

LaFeO3 (LFO) material has been widely used as a gas sensor construction material. Although LFO has been widely applied to gas sensors, the selectivity and sensitivity as well as the working temperature of gas sensors are still not optimal. The LFO in this study was Co-doped and also coated with single layer rGO to analyze its sensitivity and selectivity based on adsorption energy using Density Functional Theory (DFT). Based on this research, it was found that the presence of Co doping and rGO coating could increase the adsorption energy on the LFO. The addition of the rGO layer to the LFO increased the adsorption energy by 23.58% from -2.38 eV for Co-doped LFO to -2.93 eV when rGO was added. This shows the potential of adding rGO layers to LFO materials for sensor materials.

***Keyword** : LaFeO$_3$, Cobalt, gas sensor, ethanol, reduce graphene oxide, density functional theory*

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DAFTAR TABEL

DAFTAR GAMBAR

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