ANALISIS PENGARUH LAPISAN rGO PADA MATERIAL $LaFeO_3$ DOPING Ba SEBAGAI SENSOR GAS ETANOL MENGGUNAKAN *DENSITY FUNCTIONAL THEORY*

SKRIPSI

diajukan untuk memenuhi salah satu syarat untuk memperoleh gelar Sarjana Sains
Program Studi Fisika Kelompok Bidang Kajian Fisika Material

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PROGRAM STUDI FISIKA

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ANALISIS PENGARUH LAPISAN rGO PADA MATERIAL $LaFeO_3$ DOPING Ba SEBAGAI SENSOR GAS ETANOL MENGGUNAKAN *DENSITY FUNCTIONAL THEORY*

(Skripsi ini merupakan bagian dari payung penelitian Prof. Dr. Endi Suhendi, M.Si)

Oleh

Siti Intan Cahya Kemuning

Diajukan untuk memenuhi sebagian syarat untuk memperoleh gelar Sarjana Sains pada Fakultas Pendidikan Matematika dan Ilmu Pengetahuan Alam

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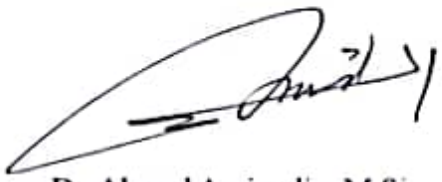

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Dengan ini saya menyatakan bahwa skripsi dengan judul "**Analisis Pengaruh Lapisan rGO pada Material $LaFeO_3$ Doping Ba Sebagai Sensor Gas Etanol Menggunakan *Density Functional Theory***" ini beserta seluruh isinya adalah benar-benar karya saya sendiri. Saya tidak melakukan penjiplakan atau pengutipan dengan cara-cara yang tidak sesuai dengan etika ilmu yang berlaku dalam masyarakat keilmuan. Atas pernyataan ini, saya siap menanggung risiko apabila di kemudian hari ditemukan adanya pelanggaran etika keilmuan atau ada klaim dari pihak lain terhadap keaslian karya saya ini.

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KATA PENGANTAR

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ABSTRAK

LaFeO3 (LFO) merupakan material yang banyak digunakan untuk membuat sensor gas dengan mekanisme adsorpsi oksigen. Sensor gas etanol untuk material LFO tidak ideal dari segi sensitivitas, selektivitas, dan temperatur kerja. Dalam penggunaan sensor gas, doping barium (Ba) umumnya digunakan untuk meningkatkan pengindraan sensor gas. Selain itu, material *reduksi Oksida Graphene* (rGO) juga banyak digunakan untuk meningkatkan kepekaan gas-sensing yang lebih baik dan kinerja respon yang cepat untuk sensor gas. Penelitian ini menggunakan Density Functional Theory (DFT) untuk melihat bagaimana doping Ba dan penambahan lapisan rGO pada material LBFO mempengaruhi energi celah pita dengan molekul gas etanol. Hasilnya menunjukkan bahwa adanya doping Ba dan lapisan rGO satu lapisan dapat meningkatkan energi adsorpsi dan energi celah pita. Penambahan lapisan rGO menunjukkan bahwa energi adsorpsi meningkat dari -2,95 eV menjadi -3,27 eV. Begitupun dengan energi celah pita LBFO penurunan energi celah pita dari 3,65 eV menjadi 2,71 eV menunjukkan interaksi kuat dengan etanol. LBFO@rGO menjadikan energi celah pita yang sangat rendah sebelum terpapar etanol sebesar 0,15 eV maupun setelah terpapar etanol sebesar 0,08 eV. Energi celah pita yang sempit menunjukkan bahwa rGO meningkatkan konduktivitas material dan mengoptimalkan struktur elektronik untuk interaksi dengan etanol. Perubahan nilai celah energi ini menunjukkan bahwa telah terjadi mekanisme adsorpsi-oksidasi pada sistem yang didukung oleh adanya data energi adsorpsi. Mekanisme adsorpsi oksidasi merupakan mekanisme dasar untuk sensor gas dapat bekerja. Dengan adanya mekanisme ini, LBFO@rGO dapat dijadikan kandidat untuk aplikasi sensor gas, terutama untuk gas aseton.

Kata Kunci: $LaFeO_3$, barium, *reduce graphene oxcide* (rgo), *density functional theory,* sensor gas, gas etanol, energi celah pita

ABSTRACT

LaFeO3 (LFO) is a material widely used for gas sensors based on the oxygen adsorption mechanism. Ethanol gas sensors using LFO are not ideal in terms of sensitivity, selectivity, and operating temperature. In gas sensor applications, barium (Ba) doping is commonly used to enhance gas sensing. Additionally, reduced Graphene Oxide (rGO) is often used to improve gas sensing sensitivity and response performance. This study employs Density Functional Theory (DFT) to investigate how Ba doping and the addition of an rGO layer on LBFO material affect the bandgap energy in the presence of ethanol gas molecules. The results show that Ba doping and a single layer of rGO can increase adsorption energy and bandgap energy. The addition of the rGO layer increases the adsorption energy from -2.95 eV to -3.27 eV. Similarly, the bandgap energy of LBFO decreases from 3.65 eV to 2.71 eV, indicating strong interaction with ethanol. LBFO@rGO exhibits a very low bandgap energy before ethanol exposure of 0.15 eV and after ethanol exposure of 0.08 eV. The narrow bandgap energy indicates that rGO enhances the material's conductivity and optimizes the electronic structure for interaction with ethanol. These changes in bandgap energy values suggest an adsorption-oxidation mechanism in the system, supported by adsorption energy data. The adsorption-oxidation mechanism is fundamental for gas sensors to function. With this mechanism, LBFO@rGO can be considered a candidate for gas sensor applications, particularly for acetone gas.

Keywords: LaFeO3, barium, reduced graphene oxide (rGO), density functional theory, gas sensor, ethanol gas, bandgap energy

DAFTAR ISI

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