

**KARAKTERISTIK MATERIAL Ag-LaFeO_3 DILAPISI rGO SEBAGAI
SENSOR GAS ETANOL MENGGUNAKAN KOMPUTASI *DENSITY*
*FUNCTIONAL THEORY***

SKRIPSI

Diajukan untuk memenuhi salah satu syarat untuk memperoleh gelar Sarjana
Sains Program Studi Fisika



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FAKULTAS PENDIDIKAN MATEMATIKA DAN ILMU PENGETAHUAN ALAM
UNIVERSITAS PENDIDIKAN INDONESIA
2024**

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Universitas Pendidikan Indonesia
Juli 2024

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**KARAKTERISTIK MATERIAL Ag-LaFeO₃ DILAPISI rGO SEBAGAI
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*FUNCTIONAL THEORY***

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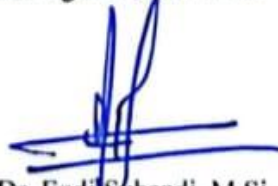


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KATA PENGANTAR

Ungkapan rasa syukur dan puji kepada Tuhan Yang Maha Esa penulis panjatkan atas limpahan rahmat, petunjuk, dan kuasa-Nya sehingga penulisan proposal skripsi dengan judul “Karakteristik Material Ag-LaFeO₃ Dilapisi rGO Sebagai Sensor Gas Etanol Menggunakan Komputasi *Density Functional Theory*” dapat diselesaikan. Skripsi ini disusun sebagai bagian dari persyaratan untuk memperoleh gelar Sarjana Sains dari Departemen Pendidikan Fisika, Program Studi Fisika.

Penulis menyadari bahwa proposal skripsi ini tidak lepas dari kekurangan dan keterbatasan. Oleh karena itu, setiap kritik dan saran yang membangun dari pembaca akan menjadi masukan berharga untuk perbaikan di masa yang akan datang. Semoga skripsi ini dapat memberikan kontribusi dan pengetahuan tambahan, khususnya dalam konteks analisis perhitungan energi adsorpsi molekul gas etanol pada material sensor gas yang dilapisi rGO. Penulis berharap agar hasil penelitian ini dapat bermanfaat bagi pengembangan ilmu pengetahuan di bidang ini. Akhir kata, penulis mengucapkan terima kasih atas dukungan dan bimbingan yang diberikan oleh semua pihak selama proses penulisan skripsi ini.

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UCAPAN TERIMA KASIH

Penyusunan skripsi ini tidak dapat berjalan dengan baik tanpa adanya motivasi, dukungan, bantuan, dan bimbingan dari berbagai pihak. Pada kesempatan ini, penulis ingin mengucapkan rasa terima kasih dengan segala kerendahan hati dan penuh rasa hormat kepada pihak-pihak yang telah memberikan doa serta dukungannya sehingga penulisan skripsi ini dapat terselesaikan, khususnya kepada:

1. Bapak Prof. Dr. Endi Suhendi, M.Si., selaku Dosen Pembimbing I dan Ketua Program Studi Fisika, yang telah memberikan bimbingan, arahan, dan motivasi kepada penulis sehingga skripsi ini terselesaikan.
2. Ibu Dr. Selly Feranie, M.Si., selaku Dosen Pembimbing II yang telah memberikan dukungan kepada penulis atas penelitian ini.
3. Ibu Prof. Dr. Lilik Hasanah, S.Si., M.Si., selaku Pembimbing Akademik yang telah memberikan arahan dan motivasi selama masa perkuliahan.
4. Badan Riset Inovasi dan Nasional (BRIN), yang menyediakan layanan komputasi yang digunakan dalam penelitian ini
5. Kedua orang tua dan kedua adik penulis yang sangat pengertian dan senantiasa memberi dukungan kepada penulis
6. Rekan-rekan penelitian sensor gas, yang saling memberikan motivasi dan teman berdiskusi selama penelitian ini.
7. Teman kelas seperjuangan, Ajriel, Aghisna, Revanya, Arik, Bagus yang telah menjadi tempat untuk bertukar pikiran selama perkuliahan.
8. Semua pihak yang tidak dapat penulis sebutkan satu per satu, yang telah memberikan bantuan dan dukungan dalam berbagai bentuk.

Semoga segala bantuan, dukungan, dan doa yang telah diberikan mendapatkan balasan yang setimpal dari Tuhan Yang Maha Esa. Akhir kata, penulis berharap semoga skripsi ini dapat memberikan manfaat bagi kita semua serta dapat menjadi kontribusi yang berguna dalam perkembangan ilmu pengetahuan dan teknologi.

ABSTRAK

Perkembangan industri dalam bidang kimia, manufaktur, dan energi mendorong kebutuhan akan piranti yang dapat mendeteksi keberadaan suatu gas yang berbahaya. Oleh karena itu, penelitian tentang semikonduktor metal oksida (MOS) dan material dua dimensi menjadi topik yang banyak dipelajari sebagai material sensor gas. LaFeO_3 yang didoping Ag (ALFO) dikenal sebagai komposisi yang baik bagi material sensor gas. Disisi lain, *Reduced Graphene Oxide* (rGO) juga menjadi material yang banyak digunakan untuk peningkatan performa sensor gas. Penelitian ini membahas efek penambahan lapisan rGO pada ALFO terhadap energi adsorpsi molekul etanol dan energi celah pita melalui studi komputasi *Density Functional Theory* (DFT). Hasil perhitungan energi adsorpsi pada ALFO dan ALFO@rGO berturut-turut diperoleh dengan nilai -4,51eV dan -6.04eV, sedangkan untuk energi celah pita sebesar 0,73eV dan 0,58eV. Hal tersebut menunjukkan bahwa material ALFO@rGO memiliki potensi yang baik sebagai sensor gas etanol.

Kata kunci: sensor gas, LaFeO_3 , doping Ag, *Reduced Graphene Oxide*, *Density Functional Theory*, etanol.

ABSTRACT

The development of industries in the fields of chemistry, manufacturing, and energy drives the need for devices that can detect the presence of hazardous gases. Therefore, research on Metal Oxide Semiconductor (MOS) and two-dimensional materials has become a widely studied topic for gas sensor materials. Ag-doped LaFeO_3 (ALFO) is known as a good composition for gas sensor materials. On the other hand, Reduced Graphene Oxide (rGO) is also widely used to enhance the performance of gas sensors. This study discusses the effect of adding an rGO layer on ALFO on the adsorption energy of ethanol molecules and the band gap energy through a Density Functional Theory (DFT) computational study. Adsorption energy calculations for ALFO and ALFO@rGO resulted in values of -4.51 eV and -6.04 eV, respectively, while the band gap energies were 0.73 eV and 0.58 eV. These findings indicate that ALFO@rGO material has good potential as an ethanol gas sensor.

Keywords: gas sensor, LaFeO_3 , Ag doping, Reduced Graphene Oxide, Density Functional Theory, ethanol.

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