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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PROGRAM STUDI FISIKA

FAKULTAS PENDIDIKAN MATEMATIKA DAN ILMU PENGETAHUAN ALAM

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Program Studi Fisika
FPMIPA UPI

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

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KATA PENGANTAR

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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 discuss 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, LaFeO3, Ag doping, Reduced Graphene Oxide, Density Functional Theory, ethanol.

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