ANALISIS PENGARUH PENAMBAHAN LAPISAN rGO PADA $LaFeO_3$ DENGAN DOPING Pd MENGGUNAKAN *DENSITY FUNCTIONAL THEORY* UNTUK SENSOR GAS

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

FAKULTAS PENDIDIKAN MATEMATIKA DAN ILMU PENGETAHUAN ALAM

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PERNYATAAN

Dengan ini saya menyatakan bahwa skripsi dengan judul "ANALISIS PENGARUH PENAMBAHAN LAPISAN rGO PADA $LaFeO_3$ DENGAN DOPING Pd MENGGUNAKAN *DENSITY FUNCTIONAL THEORY* UNTUK SENSOR GAS" ini beserta seluruh isinya adalah benar-benar karya 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/sanksi apabila di kemudian hari ditemukan adanya pelanggaran etika keilmuan atau ada klaim dari pihak lain terhadap keaslian karya saya ini.

Bandung, Juli 2024

Yang membuat pernyataan

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KATA PENGANTAR

Segala puji dan rasa syukur dipanjatkan kepada Allah SWT atas segala rahmat dan karunia-Nya, skripsi dengan judul "Analisis Pengaruh Penambahan Lapisan rGO Pada $LaFeO_3$ Dengan Doping Pd Menggunakan *Density Functional Theory* Untuk Sensor Gas" dapat diselesaikan dengan baik.

Skripsi ini telah disusun sebagai syarat untuk memenuhi mencapai gelar Sarjana Sains Fisika (S1) dari program studi Fisika, Fakultas Pendidikan Matematika dan Ilmu Pengetahuan Alam, Universitas Pendidikan Indonesia. Penulis menyadari bahwa skripsi ini masih memiliki kekurangan dan jauh dari sempurna. Oleh karena itu, kritik dan saran dari berbagai pihak akan sangat membangun untuk penulisan skripsi ini. Semoga skripsi ini dapat bermanfaat bagi para pembaca dan mendorong penelitian selanjutnya. Akhir kata, penulis mengucapkan terima kasih.

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ABSTRAK

Etanol merupakan salah satu jenis alkohol yang mudah menguap dan terdapat dampak negatif bagi kesehatan dan lingkungan sehingga diperlukan pengembangan komponen penginderaan gas etanol yaitu sensor gas. $LaFeO_3$ merupakan material perovskite ABO_3 yang banyak diaplikasikan pada sensor gas karena komposisi materialnya dan stabilitas parameter penginderaannya. Namun, $LaFeO_3$ masih terbatas sifat penginderaan gasnya sehingga diperlukan *doping* dalam peningkatan kinerja sensor gas yaitu Paladium. Selain itu, ditambahkan juga lapisan rGO untuk memperkuat energi adsorpsi. Pada penelitian ini dilakukan proses *Density Functional Theory* (DFT) dengan metode SCF, vc-relax, *bands*, serta *post-processing bands*. Hasil dari energi adsorpsi molekul gas etanol pada Pd-$LaFeO_3$ -2,01 eV dan Pd-$LaFeO_3$@rGO -2,29 eV. Penambahan rGO diketahui meningkatkan energi adsorpsi (negatif). Kemudian, untuk nilai *band gap* Pd-$LaFeO_3$ sebelum terpapar gas 2,34 eV dan saat terpapar 2,06 eV. Kemudian, Pd-$LaFeO_3$@rGO sebelum terpapar sekitar 0,11 eV dan saat terpapar 0,05 eV. Penyempitan struktur pita energi membuat nilai energi celah pita mengecil akibat terciptanya banyak *hole*. Dari hasil perubahan antara energi adsorpsi dan celah pita diketahui bahwa penambahan rGO pada Pd-$LaFeO_3$ potensial untuk dijadikan kandidat aplikasi sensor gas dari sisi kuatnya adsorpsi dan rendahnya *band gap*.

Kata Kunci : Sensor gas, $LaFeO_3$, Palladium, *reduce graphene oxide, density functional theory*

ABSTRACT

Ethanol is a type of volatile alcohol that poses negative effects on health and the environment, necessitating the development of ethanol gas sensing components, namely gas sensors. $LaFeO_3$ is a perovskite ABO_3 material commonly used in gas sensors due to its material composition and stable sensing parameters. However, $LaFeO_3$ has limited gas sensing capabilities, requiring enhancement through doping with Palladium to improve sensor performance. Additionally, an rGO layer is added to strengthen adsorption energy. This study employed Density Functional Theory (DFT) using SCF, vc-relax, bands, and post-processing bands methods. The results showed ethanol gas molecule adsorption energy on Pd-$LaFeO_3$ was -2,01 eV and on Pd-$LaFeO_3$@rGO was -2,29 eV. The addition of rGO is known to increase (negative) adsorption energy. Furthermore, the band gap of Pd-$LaFeO_3$ before gas exposure was 2,34 eV and 2,06 eV when exposed. For Pd-$LaFeO_3$@rGO, the band gap was around 0,11 eV before exposure and 0,05 eV when exposed. The narrowing of the energy band structure reduced the band gap value due to the creation of more holes. The results indicate that adding rGO to Pd-$LaFeO_3$ is a promising candidate for gas sensor applications, given its strong adsorption and low band gap.

Keywords: Gas sensor, LaFeO3, Palladium, reduced graphene oxide, density functional theory

DAFTAR ISI

DAFTAR GAMBAR

DAFTAR TABEL

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