PENGARUH LAPISAN rGO PADA $LaFeO_3$ YANG DI-*DOPING* Mn TERHADAP ENERGI ADSORPSI MOLEKUL ETANOL MENGGUNAKAN *DENSITY FUNCTIONAL THEORY*

SKRIPSI

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

oleh

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PROGRAM STUDI FISIKA
FAKULTAS PENDIDIKAN MATEMATIKA DAN ILMU PENGETAHUAN ALAM
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FPMIPA UPI

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PERNYATAAN

Dengan ini saya menyatakan bahwa skripsi dengan judul "Pengaruh Lapisan rGO pada $LaFeO_3$ yang di-*doping* Mn Terhadap Energi Adsorpsi Molekul 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.

Bandung, Desember 2023

Yang membuat pernyataan

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KATA PENGANTAR

Puji dan syukur kehadirat Tuhan Yang Maha Esa telah melimpahkan rahmat dan karunia-Nya sehingga skripsi dengan judul "Pengaruh Lapisan rGO pada $LaFeO_3$ yang di-*doping* Mn terhadap Energi Adsorpsi Molekul Etanol Menggunakan *Density Functional Theory*" dapat diselesaikan.

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ABSTRAK

$LaFeO_3$ (LFO) telah banyak diaplikasikan sebagai material penyusun sensor gas. Namun, resistansi pada material LFO masih sangat tinggi serta nilai sensitivitas dan selektivitas yang rendah. *Doping* pada LFO dilakukan untuk meningkatkan sensitivitas dan selektivitas sensor gas. Penambahan lapisan *monolayer* juga digunakan untuk mendapatkan kepekaan *gas-sensing* yang lebih baik dan kinerja respon yang cepat. Pada penelitian ini, dilakukan komputasi berbasis *Density Functional Theory* (DFT) untuk analisis pengaruh lapisan *reduced graphene oxide* (rGO) pada LFO yang di-*doping* Mangan (Mn) terhadap energi adsorpsi molekul etanol sebagai material sensor gas etanol. Berdasarkan penelitian ini, diperoleh bahwa adanya *doping* Mn dan *monolayer* rGO dapat meningkatkan energi adsorpsi. Energi adsorpsi molekul etanol terhadap sistem LFO yang di-*doping* Mn tanpa lapisan rGO bernilai -3.93 eV dan setelah adanya penambahan lapisan rGO bernilai -4.35 eV; hal ini menunjukkan eskalasi energi sekitar 10.68%. Dengan terjadinya peningkatan tersebut, proses adsorpsi pada sistem LFO yang di-*doping* Mn dan dilapisi rGO terhadap molekul etanol menjadi semakin kuat, sehingga menjadi potensial untuk dijadikan sebagai material sensor gas etanol.

Kata kunci: *density functional theory*, etanol, $LaFeO_3$, Mangan, *reduced graphene oxide*, sensor gas.

ABSTRACT

$LaFeO_3$ (LFO) is a material that has been widely applied as a material for gas sensors. However, the resistance of the LFO material is still very high, also the sensitivity and selectivity values are low. Doping on the LFO is carried out to increase the sensitivity and selectivity of the gas sensor. The addition of a monolayer is also used to obtain better gas-sensing sensitivity and fast response performance. In this research, Density Functional Theory (DFT) based computing was carried out to analyze the effect of the reduced graphene oxide (rGO) layer on Manganese (Mn) doped LFO on the adsorption energy of ethanol molecules as an ethanol gas sensor material. This research found that Mn doping and a monolayer of rGO can increase the adsorption energy. The adsorption energy of ethanol molecules on the Mn-doped LFO system without the rGO layer is -3.93 eV, and after the addition of the rGO layer, it is -4.35 eV; this shows an energy escalation increase of around 10.68%. With this increase, the adsorption process in the Mn-doped and rGO-coated LFO system towards ethanol molecules becomes more robust, so it has the potential to be used as an ethanol gas sensor material.

Keywords: density functional theory, ethanol, $LaFeO_3$, Manganese, reduced graphene oxide, gas sensor.

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DAFTAR LAMPIRAN

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