INTISARI

KAJIAN SIFAT ELEKTRONIK DAN OPTIK *TWISTED BILAYER HYDROGENATED GRAPHENE* DENGAN SUDUT UNTIRAN 30° MENGGUNAKAN METODE *TROTTER-SUZUKI TIGHT BINDING-TIME PROPAGATION*

Oleh

SYARIF MAHMUD JAILANI

23/530209/PPA/06719

Telah dilakukan kajian simulasi komputasi pengaruh adsorpsi hidrogen terhadap sifat elektronik dan optik *Twisted Bilayer Hydrogenated Graphene* dengan sudut untiran 30° (TBHG30), menggunakan pendekatan *tight binding–time propagation* (TB-TPM) berbasis dekomposisi Trotter-Suzuki. Simulasi dilakukan pada rentang konsentrasi hidrogen 0% hingga 100% untuk mengevaluasi perubahan *Density of States* (DOS) dan *optical conductivity* sebagai respons terhadap adsorpsi atom hidrogen. Pada konsentrasi hidrogen rendah, dari data DOS, struktur semimetalik *graphene* mulai terdeformasi dengan penurunan puncak singularitas Van Hove dan kenaikan *midgap states* pada level Fermi. Selain itu juga terdapat puncak-pucak di antara nilai E/t $\pm 0{,}2 \sim 1{,}2$ yang disebabkan oleh keberadaan *flat band* di sekitar level Fermi. Hal ini juga terlihat pada hasil perhitungan *optical conductivity*. Pada hidrogenasi tinggi, sistem menunjukkan transisi dari konduktor menuju semikonduktor yang ditandai oleh gap pada DOS di sekitar energi Fermi dan konduktivitas optik yang nol pada frekuensi rendah. Efek *twist* memperbesar dampak pengotor hidrogen dengan meningkatkan sensitivitas terhadap gangguan lokal, sehingga menyebabkan delokalisasi elektron terhambat secara signifikan. Interaksi antar-lapisan dihitung secara geometris berdasarkan orientasi sudut lokal atom, menjadikan model ini lebih realistis. Pendekatan Trotter-Suzuki terbukti efisien dalam menangani sistem skala besar tanpa proses diagonalisasi penuh, serta mampu menggambarkan dinamika waktu sistem dengan presisi tinggi.

Kata Kunci: *Twisted Hetero-Bilayer*, *Hydrogenated Graphene*, Metode Trotter-Suzuki, Konduktivitas Optik

ABSTRACT

STUDY OF ELECTRONIC AND OPTICAL PROPERTIES OF 30° TWISTED BILAYER HYDROGENATED GRAPHENE USING THE TROTTER–SUZUKI TIGHT-BINDING TIME PROPAGATION METHOD

By

SYARIF MAHMUD JAILANI

23/530209/PPA/06719

A computational simulation study of the effect of hydrogen adsorption on the electronic and optical properties of Twisted Bilayer Hydrogenated Graphene with a twist angle of 30° (TBHG30) has been conducted, using the tight binding–time propagation (TB-TPM) approach based on the Trotter-Suzuki decomposition. Simulations were performed at a hydrogen concentration range of 0% to 100% to evaluate changes in Density of States (DOS) and optical conductivity in response to hydrogen atom adsorption. At low hydrogen concentrations, from the DOS data, the semimetallic graphene structure begins to deform with a decrease in the Van Hove singularity peak and an increase in midgap states at the Fermi level. In addition, there are also peaks between the E/t values $\pm 0{,}2 \sim 1{,}2$ caused by the presence of a flat band around the Fermi level. This can also be seen in the results of optical conductivity calculations. At high hydrogenation, the system shows a transition from conductor to semiconductor characterized by a gap in the DOS around the Fermi energy and a zero optical conductivity at low frequencies. The twist effect amplifies the impact of hydrogen impurities by increasing the sensitivity to local perturbations, causing significant inhibition of electron delocalization. The interlayer interactions are calculated geometrically based on the local angular orientations of the atoms, making the model more realistic. The Trotter-Suzuki approach is shown to be efficient in handling large-scale systems without full diagonalization, and is able to describe the time dynamics of the system with high precision.

Keywords: Twisted Hetero-Bilayer, Hydrogenated Graphene, Trotter-Suzuki Method, Optical Conductivity