Pendekatan tight binding untuk transpor elektron molekul DNA G4 dan molekul dna aperiodik = Tight binding approach for electron transport of G4 and a aperiodik DNA molecules / Vandan Wiliyanti

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Abstrak

ABSTRAK
Sifat transportasi elektron dalam molekul DNA Aperiodik dan Molekul DNA G4 telah dipelajari. Kedua molekul DNA ini, dimodelkan dengan menggunakan Hamiltonian ikatan kuat tight binding . Sifat transpor elektron dipelajari dengan menghitung probabilitas transmisi elektron menggunakan metode transfer matriks dan hamburan matriks secara bersamaan. Formalisme Landauer-B ttiker digunakan dalam menghitung karakteristik I-V molekul dari probabilitas transmisi. Pada molekul DNA Aperiodik dan DNA G4 sudah dilakukan perhitunganan untuk DNA berukuran 32 pasangan basa. Parameter perhitungan yang diperhatikan adalah gerakan sudut putar pasangan basa yang berhubungan dengan konstanta loncatan elektron antar basa melalui teori semi-empiris Slater-Koster-Harrison. Hasil perhitungan dianalisis dengan memperhatikan variasi frekuensi getar gerak memutar, temperatur, dan energi gangguan backbone. Hasil perhitungan pada molekul DNA Aperiodik dan DNA G4 menunjukkan bahwa transpor muatan DNA bergantung pada frekuensi gerak memutar pasangan antarbasa. Jika frekuensi tinggi, terjadi peningkatan arus dan probabilitas transmisi. Dan ketika temperatur ditingkatkan, probabilitas transmisi dan arus menurun dan tegangan ambang meningkat di tiap variasi frekuensi getar gerak memutar. Terakhir, jika nilai energi gangguan backbone yang diberikan semakin besar maka nilai transmisi, arus dan tegangan ambang menurun. Pada molekul DNA G4 transmisi dan kurva I-V lebih tinggi dari molekul DNA Aperiodik.
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ABSTRACT
Electron transport characteristics in G4 and Aperiodic DNA molecules have been studied. Both molecules are modelled using tight binding Hamiltonian. Electron transport characteristics are studied by calculating electron transmission probability using matrix transfer and scattering matrix methode simultaneously. Landauer B ttiker formalism is used in calculating the I V characteristics of molecules from transmission probability. The calculation in Aperiodic and G4 DNA molecules is done for 32 base pairs long DNA. Variable in the calculation is twisting motion angle of base pairs which is correlated to electron the hopping constant between bases within Slater Koster Harrison semi empirical theory. Calculation results are analyzed in variation of twisting motion frequency, temperature, and backbone disturbance energy. The calculation result in Aperiodic and G4 DNA molecules shows that DNA change transport on DNA depends on twisting motion frequency of bases. When the frequency become higher, the current and transmission probability will increase. Moreover, when the temperature increases, the current and transmission probability decreases, then threshold the voltage becomes higher for all twisting motion frequency. Lastly, as the backbone disturbance energy become large, the current and transmission decreases, then the threshold voltage will be small. In G4 DNA molecule the transmission and curve I V are higher, than in Aperiodic DNA molecule.