Studi sifat transpor DNA: pengaruh hopping inter-strand tegak lurus pada DNA Aperiodik dan pengaruh medan listrik pada DNA G4 = Study of charge transport DNA: effect of perpendicular inter-strand hopping on Aperiodic DNA and effect of electric field on G4 DNA

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Abstrak

Sifat transpor muatan pada molekul DNA untai ganda dan DNA G4 telah dipelajari. Kami menggunakan dua model DNA yang direpresentasikan secara matematis dengan menggunakan model Hamiltonian tight binding. Model yang pertama adalah DNA untai ganda dengan panjang 32 pasangan basa yang disusun secara random. Transpor muatan untuk molekul DNA ini dipelajari dari probabilitas transmisi dan karakteristik I-V dengan memvariasikan hopping elektron inter-strand tegak lurus. Peningkatan hopping electron inter-strand tegak lurus menyebabkan probabilitas transmisi dan arus meningkat, tetapi saat temperaturnya dinaikkan probabilitas transmisi dan arus menurun. Model kedua adalah DNA G4, Sifat transpor muatan pada molekul ini dipelajari dari panjang lokalisasi dengan panjang 102 pasangan basa, density of states dan karakteristik I-V masing-masing dengan 32 tumpukan tetrad guanin, yang diberi pengaruh medan listrik dan temperatur, Probabilitas transmisi dan panjang lokalisasi dihitung menggunakan metode transfer matriks. Formula landauer Buttiker digunakan untuk menghitung karakteristik I-V. Metode fungsi green untuk menghitung probabilitas transmisi dan density of states. Hasil perhitungan medan listrik dan temperatur terhadap sifat transpor muatan yaitu menurunkan panjang lokalisasi, density of states, dan arus, saat meningkatnya medan listrik dan temperatur.

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The charge transport property on double-stranded DNA and G4 DNA molecules has been studied. We use two DNA models that are mathematically represented using Hamiltonian tight binding models. The first model is double stranded DNA with length of 32 base pairs arranged randomly. The charge transport for this DNA molecule is studied from transmission probabilities and I-V characteristics by varying of electron hopping in perpendicular inter-strand. Increased of electron hopping in perpendicular inter-strand causes the transmission and current probabilities to increase, but when temperature is increased the transmission probabilities and current is decrease. The second model is DNA G4. The charge transport property in this molecule is studied from localization length with length of 102 base pairs, density of states and I-V characteristics with 32 stacks of guanine tetrads respectively that influenced of electric field and temperature. Transmission probability and localization length are calculated using matrix transfer method. The buttiker landauer formula is used to calculate the I-V characteristics. Green function method for calculating transmission probability and density of states. The result of electric field and temperature calculation on charge transport leads to decreasing localization length, density of states, and current, when increasing of electric field and temperature.