Sifat transportasi elektron pada molekul DNA poly (dA)-poly (dT) = The properties of electron transport in poly (dA) poly (dT) DNA molecules / Kinanti Aldilla Rahmi

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Abstrak

ABSTRAK
Sifat transportasi elektron di molekul DNA poly dA -poly dT telah dipelajari. Kami menggunakan dua model DNA yang berbeda, yang direpresentasikan secara matematis dengan model ikatan kuat Hamiltonian dan teori Slater-Koster. Panjang molekul DNA yang digunakan 32 pasangan basa. Kedua ujung rantai molekul dikoneksikan dengan elektroda. Sifat transportasi elektron dipelajari dari probabilitas transmisi dan karakteristik I-V. Probabilitas transmisi dihitung dengan metode transfer matriks dan matriks hamburan. Formula Landauer Buttiker digunakan untuk menghitung karakteristik I-V. Selanjutnya, sifat transportasi elektron dibandingkan di variasi temperatur, frekuensi getar gerak memutar dan energi gangguan lingkungan luar. Hasilnya menunjukan bahwa pada kedua model mengalami peningkatan probabilitas transmisi elektron dan arus seiring meningkatnya frekuensi getar gerak memutar rantai DNA. Namun saat temperatur ditingkatkan, probabilitas transmisi dan arusnya menurun dan tegangan ambang membesar di tiap variasi frekuensi getar. Kemudian ketika energi gangguan luar meningkat, probabilitas transmisi dan arus semakin kecil, demikian pula tegangan ambangnya. Nilai puncak-puncak probabilitas transmisi di model B lebih besar dari model A, namun kurva I-V model B dapat lebih besar atau lebih kecil. Peningkatan maupun penurunan transmisi dan arus di model A lebih besar ketika tidak ada gangguan backbone, tendensi terbalik ketika terdapat energi gangguan backbone.
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ABSTRACT
The properties of electron transport in poly dA poly dT DNA molecules have been studied. We use two models of DNA which are represented mathematically by tight binding Hamiltonian model and Slater Koster theory. DNA molecules which are used have 32 base pairs long. Each end of DNA chain are connected to metallic electrodes. The properties of electron, are studied from transmission probability and I V characteristic curves. The transmission probabilities are calculated using transfer matrix and scattering matrix methods. The Landauer Buttiker formula is used in computing I V characteristics. The properties of transport electron are compared in variation of temperatures, frequencies of twisting motion and disorder energy due to environment. The results show that the transmission probability and current values increase as frequency of twisting motion increases in both of models. However, as temperature become higher, the transmission probability and current values decrease, but the treshold voltages increase for all frequency variations. Then, as disorder energy becomes higher, the transmission probability and current values decrease, and the threshold voltages decrease, too. Transmission probability values of model B are higher than model A, but the I V curve of model B can be higher and lower. Both of the enhancement or reduction of transmission and current in model A is higher for without backbone disorder energy condition, but the tendency reversed when in backbone disorder energy condition.