

1. Record Nr.	UNINA9910346861203321
Autore	Wolter Mario
Titolo	Charge Transport in DNA - Insights from Simulations
Pubbl/distr/stampa	KIT Scientific Publishing, 2013
Descrizione fisica	1 online resource (VI, 139 p. p.)
Soggetti	Chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Sommario/riassunto	Charge transport and charge transfer (CT) capabilities of deoxyribonucleic acid (DNA) are investigated. A QM/MM multi-scale framework is applied to calculate the CT capabilities of DNA under conditions resembling the experimental setup. The simulations are able to explain and predict the outcome of experiments and therefore make suggestions in advance. Based on the findings, suitable DNA sequences can be opted for the design of DNA-based devices as nano-scale electronic elements.