Sensing Organic Molecules by Charge Transfer through Aptamer-Target Complexes: Theory and Simulation

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Aptamers, i.e., short sequences of RNA and single-stranded DNA, are capable of specificilly binding objects ranging from small molecules over proteins to entire cells. Here, we focus on the structure, stability, dynamics, and electronic properties of oligonucleotides that interact with aromatic or heterocyclic targets. Large-scale molecular dynamics simulations indicate that aromatic rings such as dyes, metabolites, or alkaloides form stable adducts with their oligonucleotide host molecules at least on the simulation time scale. From molecular dynamics snapshots, the energy parameters relevant to Marcus' theory of charge transfer are computed using a modified Su-Schrieffer-Heeger Hamiltonian, permitting an estimate of the charge transfer rates [1]. In many cases, aptamer binding seriously influences the charge transfer kinetics and the charge carrier mobility within the complex, with conductivities up to the nanoampere range for a single complex. We discuss the conductivity properties with reference to potential applications as biosensors [2].

[1] T. Cramer, S. Krapf, T. Koslowski, J. Phys. Chem. B 108, 11812 (2004)
[2] M. Schill, T. Koslowski, J. Phys. Chem. B 117, 475 (2013)