

Sensing Molecules by Charge Transfer through Aptamer-Target-Complexes

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Aptamers, i.e. short sequences of RNA and single-stranded DNA, are capable of specifically 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 alkaloids form stable adducts with their oligonucleotide host molecules at least on the 20 ns time scale. From molecular dynamics snapshots, the energy parameters relevant to Marcus' theory [1] of charge transfer are computed using a modified Su-Schrieffer-Heeger Hamiltonian [2], permitting an estimate of the charge transfer rate, k_s , through the whole system. 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. As a consequence, these adducts constitute a new class of model systems that enable the investigation of macromolecular charge transfer with potential applications as nanoscopic single-molecule sensors [3].

[1] R. A. Marcus, *J. Chem. Phys.*, **1956**, *24*, 966-978.

[2] W. P. Su, J. R. Schrieffer, A. J. Heeger, *J. Phys. Rev.*, **1980**, *22*, 2099-2111.

[3] M. Schill, T. Koslowski, *J. Phys. Chem.*, **2013**, *117* (2), 475-483.