Electrostatics of DNA-Functionalized Nanoparticles

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functionalized nanoparticles have applications in directed self-assembly and targeted
cellular delivery of therapeutic proteins. In order to design specific systems, it is
necessary to understand their self-assembly properties, of which the long-range elec-
trostatic interactions are a critical component. We iteratively solved equations de-
derived from classical density functional theory in order to predict the distribution of
ions around DNA-functionalized Cg Catalase. We then compared estimates of the
resonant intensity to those from SAXS measurements to estimate key features of
DNA-functionalized proteins, such as the size of the region linking the protein and
DNA and the extension of the single-stranded DNA. Using classical density func-
tional theory and coarse-grained simulations, we are able to predict and understand
these fundamental properties in order to rationally design new biomaterials.

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