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Electrostatics of DNA-Functionalized Nanoparticles KYLE HOFFMANN, KURINJI KRISHNAMOORTHY, SUMIT KEWALRAMANI, MICHAEL BEDZYK, MONICA OLVERA DE LA CRUZ, Northwestern University — DNA-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 electrostatic interactions are a critical component. We iteratively solved equations 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 functional 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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