Abstract Submitted
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Local Ionic Environment around Polyvalent Nucleic-Acid Functionalized Gold Nanoparticles[1] MONICA OLVERA DE LA CRUZ, JOS ZWANIKKEN, Department of Materials Science and Engineering, Northwestern University, CHAD MIRKIN, Department of Chemistry, Northwestern University — Polyvalent oligonucleotide-functionalized gold nanoparticles (DNA-AuNPs) are remarkably stable in a cellular environment against degradation by nucleases, a property that was recently attributed to the local high concentration of mono- and divalent ions (Ref 1). In order to evaluate this hypothesis, we investigated the composition of the ion cloud around spherical nanoparticles that are functionalized by stiff, highly charged polyelectrolyte chains by means of classical density functional theory and molecular dynamics simulations. We developed a cell model that includes ligands explicitly and both applies over the entire relevant parameter space and is in excellent quantitative agreement with simulations (Ref 2). The ion distribution around the DNA-AuNPs as a function of DNA grafting densities and bulk ionic concentrations, as well as different sizes of nanoparticles and chains, is studied. For small particles with high DNA surface densities, we find strongly enhanced local salt concentrations, a pronounced localization of divalent ions near the surface of the nanoparticle, and a large radial component of the electric field between the ligands. Therefore, we conclude that enzyme activity in general may be heavily influenced by the local environment around DNA-AuNPs.

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Ref 1: A. E. Pelling, et al. Science 332, 217 (2009). Ref 2: J. W. Zwanikken, et al. J. Phys. Chem. C 115 (33), 16368 (2011)

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