

Abstract Submitted  
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**Fundamental Interactions between Deoxyribonucleic Acid (DNA) Oligomers and Au Nanoparticles: Experimental and Theoretical Studies** MOLLESHREE KARNA, Science and Math Academy, Aberdeen High School, Aberdeen, MD 2100, Army Research Lab, Aberdeen Proving Ground, MD 21005, RADHAKRISHNAN BALU, MARK GRIEP, GOVIND MALLICK, Army Research Lab, Aberdeen Proving Ground, MD 21005 — Experimental and theoretical investigations were performed to understand the nature of fundamental interactions between gold nanoparticles (GNPs) and single stranded DNA (ss-DNA). Atomic force microscopic imaging and UV-Visible spectroscopic measurements revealed binding of NPs with ss-DNA under mildly acidic conditions.. *Ab initio* quantum chemical calculations within the framework of density functional theory provided a possible charge transfer pathway from the DNA base guanine to Au atoms and thus characterizing the interaction as electrostatic. The calculations outline the possible effect of the presence of other bases to guanine mediated charge transfer. Specifically, the presence of an adenine base alters the charge localization at the guanine base and thus prevents charge transfer to NPs.

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