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Ab Initio Calculation of Structural Photophysical Properties of Cytosine and Guanine Ligated Ag cluster MOHAMMED JABED, NAVEEN DANDU, SVETLANA KILINA, North Dakota State University — DNA relaxed small silver is considered a promising new type of fluorophore for various application due to its exhibition of bright emission from visible to near-infrared range. Single strand DNA synthesized silver cluster has fluorescence properties and it has been shown distinct photophysical properties when linked through DNA strand and formed a dimer. Mechanism of dimer formation, electrochemical and photophysical properties of Ag cluster is still unknown. We have performed Density Functional Theory (DFT) calculations to optimize varying sizes of the silver cluster with different nucleotide ligands. We also made Ag dimer by the different mechanism and optimized by DFT method. Calculated electrochemical properties show that redox potential is dependent on the cluster size and spin state of the system as well. We have performed Time Dependent DFT (TD-DFT) for all monomer and dimer. It has shown that absorption of a monomer depends on size and charge of the cluster. On the other hand, partial replacement of cytosine by guanine could increase the intensity of lower energy band. We made conjugate bridged dimer to study any possible charge transfer nature of Ag clusters. We have found that dimer absorption could be red shifted due to conjugation bridge and size independent absorption of doublet spin system.

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