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by

Pushotam Sharma, Sitansh Sharma, Abhijit Mitra, Harjinder Singh

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Centre for Computational Natural Sciences and Bioinformatics
International Institute of Information Technology
Hyderabad - 500 032, INDIA
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A Theoretical Study on Interaction of Small Gold Clusters $\text{Au}_n$ ($n = 4, 6, 8$) with xDNA Base Pairs

Purshotam Sharma, Sitansh Sharma, Abhijit Mitra and Harjinder Singh

Center for Computational Natural Sciences and Bioinformatics, International Institute of Information Technology, Hyderabad, 500032, India

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Abstract

xDNA constitutes a novel class of size expanded synthetic nucleic acids in which one of the bases of the base pairs is larger than the natural DNA bases. These expanded bases are called x-bases. In this paper, we investigate the hydrogen bonding characteristics and relevant molecular properties of model complexes $(\text{xA} \cdots \text{T})$–$\text{Au}_n$, $(\text{xT} \cdots \text{A})$–$\text{Au}_n$, $(\text{xG} \cdots \text{C})$–$\text{Au}_n$, and $(\text{xC} \cdots \text{G})$–$\text{Au}_n$ ($n = 4, 6, 8$) consisting of xDNA base pairs and gold clusters, in order to study the nature of gold-xDNA binding. We offer detailed characterization of their different aspects, viz., structural, electronic and spectroscopic, effect of gold cluster size, aromaticity, and planarity using quantum mechanics based density functional theory (DFT). Significant charge transfer is seen between the gold clusters and x-base pairs. Gold complexation is found to affect the interbase hydrogen bonding in these complexes. In addition to anchor bonds, $\text{X} \cdots \text{H} \cdots \text{Au}$ type of hydrogen bonding interactions are also found to contribute to the gold-base pair binding in these complexes.