

Abstract Submitted
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Stereochemical and Thermodynamic Analysis of Biochemical Nanoparticles as Contrast Agents For Bio Imaging¹ SI YOUNG CHOI, Brooks School, ANDREW KYUNG, Northern Valley Regional High School at Demarest — Contrast agents are crucial in medical imaging, effectively improving the clarity and contrast of the targeted body part. Clear differentiation between the body structure and nearby tissue is necessary for accurate clinical examination and diagnosis. Through empirical and computational research, image contrast agents that are higher in stability and safety are examined. Magnetic resonance imaging, a major diagnostic method in modern medicine, is safe due to the absence of damaging ionizing radiation. Researchers have used electrochemical techniques to study aqueous fullerene nanoparticles as not only X-Ray contrast agents, but also MRI contrast agents. This paper uses computational simulations to examine the potential of nanomaterials such as fluorescent functionalized Gadolinium and metal oxides to be used as nano-scaled contrast agents in the detection of tumor cells. The paper presents the analysis and comparison of thermodynamic stability of various imaging contrast agents, such as derivatives of lanthanide element and metal oxides by assessing the optimized energy via chemical programs. The electron properties of contrast agents are examined by Density Functional Theory (DFT) and Universal Force Field (UFF) method which employ quantum physical and chemical method.

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