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Study of the Contrast Agents Containing Metal Oxides and Lanthanide Element for Bioimaging MIN JAE SHIN, RICHARD KYUNG, Choice Research Group — The unique magnetic properties of the gadolinium ion allowed it to be used in a variety of ways, especially in MRI scanning. However, the use of some Gd(III) chelates in persons with renal disease was linked to a rare but severe complication, which may occur months after contrast has been injected. The common use of iodinated molecules as contrast agents has potential drawbacks, such as high dosage that lead to toxicity and lack of stability, motivating researchers to seek for alternatives that could yield more efficient results. Fluorescent functionalized fullerenes, metal oxide nanoparticles, such as titanium oxide and tantalum oxide have been on a rise as cost-efficient and biocompatible contrast agents in the medical world. In this paper, computational studies using program softwares and Density Functional Theory (DFT) for the functionalized molecules and metal oxides were used to determine whether fluorescent molecules are suitable contrast agents to use. The molecules were modeled and the safety and stability were checked quantitatively by analyzing the optimized energies of the molecules.

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