INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Programme of Study : **Ph.D.**

Thesis Title: **Computational Exploration of 3d and 4f Metal Complexes Relevant to Magnetic Resonance Imaging and Molecular Magnetism**

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SHORT ABSTRACT

This thesis primarily focuses on the computational investigation of the atomistic behavior of Ln^{3+} (Ln=La^{3+}, Gd^{3+}, and Lu^{3+}) and Mn^{2+} complexes corresponding to their unique electronic and magnetic properties. Accordingly, *ab initio* molecular dynamics (AIMD) simulations were carried out to investigate the structural dynamics of these complexes at varying temperatures. Additionally, the thermodynamic stability is analyzed through the Gibbs free energy of formation of the complexes. A key factor in MRI CAs is optimizing the water exchange rate (k_{ex}^{298}) of the coordinated water molecules with bulk water, as it directly influences relaxivity. The interaction between water molecules and metal ions has been evaluated using quantum chemical methods, providing insights into the water exchange kinetics. In the realm of molecular magnetism, the magnetic anisotropy of Mn^{2+} complexes is determined through the analysis of the axial zero-field splitting (ZFS) parameter (D). Variations in the ligand environment markedly influence both the axial (D) and rhombic (E) components of the zero-field splitting (ZFS) parameters, thereby modulating the electronic relaxation processes in MRI contrast agents and the overall magnetic behavior of the complexes. These insights are expected to guide the rational design of next-generation diagnostic and therapeutic agents for biomedical applications, as well as advanced materials for data storage technologies.