INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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

Thesis Title: **Crystalline Molecular and Nanoparticle Assemblies with Optoelectronic Application Potential**

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Thesis Submitted to the Department/ ~~Center~~	:	Chemistry
Date of completion of Thesis Viva-Voce Exam	:	19-06-2024
Key words for description of Thesis Work	:	SERS, Molecular Crystals, Phosphorescence, Nanomaterials

SHORT ABSTRACT

The current thesis describes the production and prospective use of molecular crystals and crystallization-induced nanomaterial assembly. The current thesis reveals that the surface of molecular crystals can serve as an appropriate SERS platform. The surface functionality of molecular crystals can participate in non-covalent interactions with the deposited analyte molecules, allowing for efficient photoinduced charge transfer. The current thesis also shows that inorganic molecular crystals can exhibit metallic characteristics and cause surface plasmon. These molecular crystals may be exploited as a possible SERS substrate due to their excellent spectrum stability, simplicity of synthesis, outstanding environmental stability, biocompatibility, target molecule selectivity, and molecular cooperativity. The thesis also depicts the tuning of NC characteristics as a dopant inside molecular crystals, which sheds light on the methods for inducing tuneable phosphorescence features on simple metal NCs via ordered packing structures inside molecular crystals by altering the surrounding environment and electronic confinements. Furthermore, we used the intermolecular interaction-based surface complexation approach that causes molecular crystal formation to self-assemble nanomaterials into the crystalline superstructure.

The thesis is divided into six chapters, with the kernel of each underlined below.

Chapter 1 surveys the literature on various features resulting from the crystalline assembly of molecules and nanomaterials, including surface properties, potential applications, and possible intermolecular interactions within the crystalline assembly.

Chapter 2 shows that a microcrystal of π-conjugated copper 8-hydroxyquinolinate (CQ) is an appropriate platform for surface-enhanced Raman scattering (SERS). We also showed that such a microcrystal possesses metallic properties along all crystallographic axes and may increase molecule-specific Raman signals through plasmonic and charge-transfer mechanisms.

Chapter 3 shows that the organic compound terephthalic acid microcrystals display molecule-specific and cooperative Raman scattering of surface-deposited analyte molecules, resulting in a million-fold signal increase. Photo-induced charge transfer transitions and the idea of hybrid orbitals via noncovalent contacts in the combined system shed light on the cooperative, molecule-specific intense SERS performance.

Chapter 4 portrays that doping inside molecular crystals can be used as a easy generalized route colour tuneable solvent-processable persistent fluorescence to phosphorescence switching at room temperature. They provide significant insight on the tunability of PL property of dopant i.e., aggregated metal nanoclusters, depending on the surrounding crystalline environment and compactness of the confinement.

Chapter 5 describes the surface complexation process between zinc ions and phosphate, which can assemble colloidal zinc oxide (ZnO) quantum dots (Qdots) into three-dimensional crystalline superstructures. Crystalline assembly was begun by the controlled growth of zinc phosphate tetrahydrate complexes across the Qdot surface, resulting in assembly formation. Crystalline networks in the ZnO Qdot-phosphate nanosensor film enhanced electron mobility across the structure, allowing for selective and sensitive electrochemical gas detection.

Chapter 6 summarises the thesis and discusses possible next directions. I have also included experimental evidence illustrating the synthesis of moiré superlattices of non-van der Waals 2D crystals as a future promise.