INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: **Molecular Moiré Superlattices for Prospective Quantum Molecular Devices**

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SHORT ABSTRACT

The current thesis focuses on the assembly of small organic molecule to molecular moiré superlattices with application potential as quantum molecular devices. The initial work in this thesis focuses on the assembly of metal complexes to form 0-dimensional nanoparticles that display size-dependent luminescent and magnetic properties. These nanoparticles can further be assembled into 2D moiré superlattices. The chapters following this work discusses the self-assembly of simple organic molecules into 2D crystalline nanosheets that further forms multilayered moiré superlattices after twisted stacking. They display extraordinary tunable physical and chemical properties depending on the molecular interaction at the twisted interface compared to their 2D counterparts. Further the twist angles and moiré periodicities can be controlled by addition of Zn^{2+} ions to moiré superlattices. The Zn-complexed moiré superlattices of tryptophan further acted as spin filters. The current thesis is divided into six chapters. The works reported in these chapters are briefly discussed below.

Chapter 1: The chapter includes a brief literature review on molecular organization to form hierarchical structures of 0, 1 and 2D crystalline assemblies and their properties based on their molecular interactions. It also includes a brief discussion of how molecules and their assemblies were proposed to be used as molecular machines and eventually became favorites in molecular electronics, spintronics and quantum molecular devices.

Chapter 2: The initial work for this dissertation focuses on the assembly of metal complexes to form 0-dimensional nanoparticles that display size-dependent luminescent and magnetic properties. These types of nanoparticles can also be further assembled into 2D moiré superlattices. This work inspired us to synthesize moiré superlattices that is assembled from simple organic molecules.

Chapter 3: The chapter introduces the concept of moiré superlattice formation from small organic molecules. In this chapter, the chemical synthesis of moiré superlattices of L or D tryptophan (trp) molecules are described that were formed by the twisted stacking of the self-assembled crystalline 2D nanosheets in an aqueous medium that showcased new physical and chemical properties through interactions at the crystal interfaces.

Chapter 4: This chapter proposes the potential use of molecular moiré superlattices for building complex circuits, information storage, or sensing based on the principles of quantum mechanics at the molecular length scales. Further electrical properties of multilayered moiré superlattices of p-phenylenediamine were studied where it was dependent on the twist angle between two consecutive layers and pH of the medium.

Chapter 5: This chapter explores the concept of spin-polarized conductance through Zn-complexed moiré superlattices of D/L-trp and thus acted as spin filters. The twist angles and moiré periodicities were controlled by addition of Zn^{2+} ions to moiré superlattices of D/L-trp.

Chapter 6: This chapter includes the summarization and the future prospects for the work presented in this thesis.