Indian Institute of Technology Delhi

School of Interdisciplinary Research (SIRe)

SIRe Project Number

2026-01-31

(will be assigned by SIRe)

Project Proposal for Ph.D.

Project Details (The research problem must clearly indicate the need for an interdisciplinary approach)	
Project Title	Deep Learning-Based Raman Spectral Interpretation for 2D Materials
Project Summary (Minimum 500 and maximum 2000 characters)	Understanding and controlling interfacial charge transfer in low-dimensional systems is central to advancing next-generation optical sensing and molecular recognition technologies. Raman spectroscopy, particularly when enhanced via surface-enhanced Raman spectroscopy (SERS) and photo-induced enhanced Raman spectroscopy (PIERS), provides a powerful route to probe such processes. However, in hybrid systems composed of plasmonic nanostructures integrated with two-dimensional (2D) materials, Raman responses arise from a complex interplay of electromagnetic enhancement, chemical interactions, and photo-induced charge transfer. The resulting spectra are often highly convoluted, making conventional interpretation approaches inadequate for extracting meaningful physical insights.This project proposes an interdisciplinary framework combining advanced spectroscopy, 2D materials science, and deep learning to address this challenge. The central goal is to develop robust, data-driven models capable of decoding Raman spectra from complex hybrid systems and linking them directly to underlying charge-transfer mechanisms. A broad class of 2D materials including MXenes, transition metal dichalcogenides, graphene-based systems, and related layered materials—will be explored in conjunction with plasmonic nanoparticles (e.g., Au, Ag), forming heterostructures with tunable electronic properties. These systems enable controlled modulation of work function, interfacial band alignment, and carrier dynamics, which critically influence PIERS responses.To capture these complexities, the project will integrate experimental Raman spectroscopy, theoretical modeling (density functional theory), and state-of-the-art deep learning architectures. Machine learning models such as convolutional neural networks and physics-informed neural networks will be trained on large spectral datasets to identify hidden correlations between spectral features and physical processes, including hot electron transfer, Fermi-level equilibration, and light-driven carrier dynamics. Importantly, explainable AI approaches will be employed to ensure interpretability, enabling the extraction of physically meaningful descriptors rather than purely empirical predictions. The interdisciplinary nature of this work lies in the synergistic integration of materials design, optical spectroscopy, and artificial intelligence. Expertise from multiple domains will be combined to (i) design and synthesize tunable 2D material–plasmonic hybrids, (ii) experimentally probe their photo-induced Raman responses, and (iii) develop predictive computational models for spectral interpretation and materials optimization. This integrated strategy will ensure both fundamental understanding and practical applicability.The expected outcomes include: (i) a generalized deep learning framework for Raman spectral interpretation of complex hybrid systems, (ii) new insights into photo-induced charge transfer mechanisms at 2D interfaces, and (iii) design principles for engineering high-performance PIERS/SERS substrates. Beyond fundamental science, this work has strong implications for real-world applications, including ultrasensitive chemical sensing, environmental monitoring, and bio-diagnostics.By bridging traditionally distinct disciplines, this project aligns strongly with the vision of interdisciplinary research and aims to establish a new paradigm for data-driven spectroscopy in advanced material systems.

Ph.D. Supervisors+ (Supervisor 1 and Supervisor 2 cannot be from the same department of IITD)			
Role	**Name of Faculty**	**Academic Unit in IITD/Institute/University**	**Email ID (Official)**
Supervisor 1*	Dr. Soumik Siddantha	BCHM, IIT Delhi	soumik@iitd.ac.in,
Supervisor 2	Dr. Jayaramulu Kolleboyina	IIT Jammu	jayaramulu.kolleboyina@iitjammu.ac.in

*Supervisor 1 must be from IIT, Delhi.
+All cells in this table are mandatory fields that need to be filled by faculty for consideration of proposal.
$The date of superannuation of supervisors should be at least three years from the date of registration of selected candidates.

Project requirements (Student qualifications, experience required, etc) ***The candidate will be shortlisted based on common shortlisting criteria decided by ScRC (SIRe)**
M.Tech / M.E / M.Sc (Physics, Chemistry, Materials Science, Nanoscience, Electrical Engineering, or related areas)

Source of fellowship/funding and project number (CSIR/UGC/DBT/ICMR/ICAR/NEET-PG/DST-INSPIRE/IRD/FITT Project details, if any)
The candidate should have own funding from CSIR/UGC.

Role of Faculty Members involved:	
Supervisor-1	Expertise in *Raman spectroscopy and Machine Learning / Data-driven spectral analysis*
Supervisor-2	Expertise in *2D materials synthesis, characterization, and device applications*

Note :-

1. **Approval from the respective DRC/CRC/ScRC of your Department/Centre/School will be required for using the "Full-time Institute Assistantship (Category-wise) (FIA)" for selecting the students in SIRe.**
2. **Declaration:- Faculty members, please ensure that you have at least 3 years of service left before superannuation along with adequate sitting space & lab facilities for the SIRe student.**
3. **PI/s are also encouraged to submit joint proposals with AIIMS, NII, JNU and institutes with which IITD has an existing MoU. If the Co-PI (Supervisor 2) is from outside IITD, kindly share his/her detailed CV.**
4. **If a research scholar is to be considered for selection under the project fellowship, then the project should have a minimum of two-year duration remaining.**
5. **A candidate applying with a valid JRF/INSPIRE/any national level fellowship should have at least two-year validity from the date of joining the Ph.D. program.**
6. **The third supervisor's name (if required) can be added only after the formation of Student Research Committee (SRC) subject to a strong recommendation of SRC and subsequent approval from the competent authority.**
7. **If Institute fellowship is being sought, then DRC approval of the parent department of Supervisor 1 is required at the time of selection.**