Website Information
Department of Physics
Dayananda Sagar University

Faculty details :

Item	**Details**
Faculty Name:	Dr. Adrish Chakraborty
Room No:	Cabin No: 318
Designation:	Assistant Professor
Contact No & E-Mail	8474032160 & adrish-phy@dsu.edu.in
Research Area:	Soft condensed matter physics (Liquid crystal)

Publications (Past 5 years)	(a) A. Chakraborty, K. Garg, P. Kula, D. Bhattacharjee, A. Bhattacharjee, A Computational Exploration of 4F6T Orthoconic Antiferroelectric Liquid Crystal and Its Fluorinated Derivatives for Enhanced Nonlinear Optical Characteristics, International Journal of Thermofluids (2025), 101254. (b) A. Chakraborty, P. Kula, D. Bhattacharjee, A. Bhattacharjee, A density functional theory-based exploration of structure–property relationships in fluorinated antiferroelectric liquid crystal compounds, Discover Applied Sciences, 7 (2025), 985. (c) A. Chakraborty, K. Garg, P. Kula, D. Bhattacharjee, A. Bhattacharjee, Electronic, thermodynamic, NLO, and spectroscopic properties of OAFLC compounds via DFT: A focus on 1F6B, 1F6Bi, 1F6BiN, and 1F6BN, Journal of Molecular Liquids, 414 (2024), 126234. (d) A. Chakraborty, K. Garg, P. Kula, D. Bhattacharjee, A. Bhattacharjee, Effect of alkyl chains on the structural and optical properties of nH6BiN orthoconic antiferro-electric liquid crystals: Insights from DFT calculations, Journal of Molecular Liquids, 414 (2024), 126237. (e) A. Chakraborty, K. Garg, D. Bhattacharjee, A. Bhattacharjee, Unveiling the influence of fluorine substitution on NLO and vibrational properties: A computational exploration of N-(4-decylphenyl)-1-(4-(pentyloxy) phenyl) methanimine liquid crystal derivatives, Journal of Molecular Liquids (2024), 125101. (f) A. Chakraborty, D. Bhattacharjee, A. Bhattacharjee, Insights into the dynamic symphony: a comprehensive computational exploration of pure and fluorinated 6O.6 liquid crystals with the help of DFT analysis, Liquid Crystals (2024), 1–13. (g) A. Chakraborty, D. Bhattacharjee, A. Bhattacharjee, Exploring odd-even sensitivity in m.OnO.m liquid crystal compounds: A comprehensive study using DFT analysis, Journal of Molecular Liquids, 403 (2024), 124800. (h) A. Chakraborty, K. Garg, D. Bhattacharjee, A. Bhattacharjee, A detailed exploration of the impact of fluorination on different physical properties in 5O.12 Schiff-based liquid crystal: A DFT approach, Chemical Physics Impact, 8 (2024), 100596. (i) A. Chakraborty, D. Bhattacharjee, P.R. Alapati, A. Bhattacharjee, Theoretical investigation of N (p-nalkyloxy benzylidene) p-n alkyl aniline schiff-based liquid crystal molecule, Physics B: Condensed Matter (2024), 415857. (j) A. Chakraborty, D. Bhattacharjee, A. Bhattacharjee, Quantum Mechanical Density Functional Approach for the Studies of Nonlinear Optical and Reactivity Parameter of 5O.5 Liquid Crystal, NanoWorld Journal, 9 (2023), 227–230.

Publications (Past 5 years)	(k) K. Garg, A. Chakraborty, M. Zak, J. Herman, A. Naha, D. Bhattacharjee, Impact of fluorine substitution on benzene ring in two fluorinated liquid crystal compounds: a comprehensive analysis using TG-DTA, FT-IR, UV, and PED techniques, Discover Applied Sciences, 7 (2025), 1–39. (l) K. Garg, A. Chakraborty, A. Bhattacharjee, S.P. Choudhury, S. Kumari, D. Bhattacharjee, A DFT analysis of thermodynamical, structural and non-linear optical properties of liquid crystalline compounds (5O.m, m=14,16), Journal of Molecular Liquids, 414 (2024), 126124. (m) K. Garg, A. Chakraborty, P.R. Alapati, A. Bhattacharjee, D. Bhattacharjee, Theoretical studies and temperature-dependent Raman spectroscopy of Schiff ’s bases 5O.12 liquid crystalline compound, Journal of Molecular Structure (2024), 138867.
Profile Links : Scopus and Orcid	**Scopus ID:** 58846680300 **Orcid:** 0009-0004-3704-8638 Google Scholar: https://scholar.google.com/citations?user=aZdNUpkAAAAJ&hl=en&oi=ao

Research Activities (Write about your best research results max of 2-3 pages including diagrams)	**Research Activities** My research work is focused on the computational investigation of molecular materials, with particular emphasis on liquid crystal compounds, nonlinear optical (NLO) properties, vibrational spectroscopy, and structure–property relationships. My research combines Density Functional Theory (DFT) calculations with molecular-level electronic, vibrational, and structural analyses to understand how molecular structure and chemical substitution influence the physical properties of functional materials. **1. Density Functional Theory Studies of Liquid Crystal Materials** A major part of my research has been devoted to the theoretical investigation of calamitic and ferroelectric liquid crystal compounds. Liquid crystals are molecular materials whose properties are strongly influenced by molecular architecture, flexibility, terminal groups, linking groups, and the nature of substituents. My work has therefore focused on establishing relationships between molecular structure and properties that are relevant to the design and development of liquid crystal materials. I have carried out DFT calculations using the B3LYP functional with appropriate Gaussian basis sets, particularly 6-311G(d,p), to optimize molecular geometries and investigate the electronic and molecular properties of liquid crystal compounds. The calculations were performed for isolated molecules under standard conditions, followed by detailed analysis of the optimized structures. Gaussian 09 and GaussView have been used extensively for quantum-chemical calculations and visualization. The investigated systems include several homologous and dimeric liquid crystal series, Schiff-base liquid crystals, fluorinated compounds, and orthoconic antiferroelectric liquid crystal (OAFLC) materials. Representative systems include the nO.m series, 5O.10, 5O.12, 6O.6, 7.O3O.7–7.O8O.7, nF6R, nH6BiN, 4F6T and its fluorinated derivatives, as well as related OAFLC compounds. These studies have allowed me to examine how changes in alkyl-chain length, molecular linkage, and fluorine substitution affect molecular properties. **2. Nonlinear Optical Properties and Structure–Property Relationships** One of the important areas of my research has been the investigation of nonlinear optical properties of liquid crystal molecules. The molecular dipole moment, total and anisotropic polarizability, isotropic polarizability, and first-order hyperpolarizability have been calculated and analyzed to understand the optical response of the molecules. I have examined the relationship between molecular structure and NLO response by considering parameters such as the total dipole moment, polarizability, anisotropic polarizability, and first-order hyperpolarizability. The calculated tensor components have also been used to distinguish the molecular response along different molecular directions. These analyses provide a molecular-level interpretation of how structural modifications can influence optical properties. The results from these studies indicate that changes in molecular architecture, conjugation, terminal groups, and substitution can produce measurable changes in electronic distribution and molecular polarizability. In particular, the presence and position of electron-donating or electron-withdrawing substituents can modify charge distribution along the molecular framework, thereby affecting the calculated optical response. To complement the conventional NLO parameters, I have also investigated molecular electrostatic potential and electron-density-related properties. Such analyses help connect the calculated optical response with the underlying electronic structure of the molecules.

3. Electronic Structure and Reactivity Analysis

Another major component of my research is the analysis of molecular electronic structure. HOMO and LUMO energies and their energy separation have been evaluated for the investigated liquid crystal molecules. The HOMO–LUMO gap provides useful information about the electronic structure and possible charge-transfer characteristics of the molecular systems.

I have further used calculated electronic parameters to evaluate global chemical descriptors such as ionization potential, electron affinity, global hardness, softness, and electrophilicity. These parameters provide an additional framework for comparing molecules within a homologous series and for understanding the effect of structural modification on molecular reactivity.

Electrostatic potential (ESP) and atomic charge distributions have also been studied. In particular, atomic polar tensor (APT) charges have been used to examine charge redistribution within the molecules. These calculations provide information about the regions of positive and negative electrostatic potential and help explain the influence of different functional groups and substituents on molecular properties.

4. Vibrational Spectroscopy and Normal Mode Analysis

I have also worked extensively on the theoretical interpretation of infrared and Raman vibrational spectra of liquid crystal molecules. DFT-based vibrational frequency calculations were used to obtain the normal modes, followed by detailed assignment of the calculated vibrational bands.

The calculated vibrational spectra were analyzed in terms of molecular motions such as C–H stretching and bending, C–C and C=C stretching, C=N vibrations, aromatic ring modes, alkyl-chain vibrations, and vibrations associated with substituted functional groups. Potential energy distribution (PED) analysis using VEDA has been employed to identify the dominant internal coordinates contributing to individual normal modes.

This approach has been particularly useful for avoiding assignments based only on the visual appearance of normal modes. By combining calculated frequencies, normal-mode visualization, and PED analysis, I have been able to provide more detailed assignments of Raman and infrared bands and relate spectral features to specific molecular motions.

5. Electron Localization and Molecular Topology

To obtain a deeper understanding of chemical bonding and electron distribution, I have also used electron localization function (ELF) and localized orbital locator (LOL) analyses. These methods provide a visual description of electron localization and help identify regions associated with chemical bonds, lone-pair electrons, and localized electronic density.

The ELF and LOL analyses have been used alongside ESP and charge-distribution studies to interpret the electronic characteristics of the investigated molecules. This combination of computational tools provides a more complete picture of the relationship between molecular geometry, electron distribution, and calculated physical properties.

	6. Research on Fluorinated and Antiferroelectric Liquid Crystals A significant part of my recent research has involved fluorinated liquid crystal systems and orthoconic antiferroelectric liquid crystal materials. Fluorination is particularly interesting because the incorporation of fluorine can modify molecular polarity, electronic distribution, intermolecular interactions, and molecular anisotropy without introducing a large structural change to the molecular framework. I have investigated fluorinated derivatives of liquid crystal compounds to understand how the number and position of fluorine atoms influence molecular properties. Comparative DFT studies of different fluorination patterns have been used to examine changes in dipole moment, polarizability, hyperpolarizability, electronic structure, charge distribution, and vibrational characteristics. These studies have helped establish computational structure–property relationships within related molecular systems and provide theoretical information that can be useful when selecting or modifying liquid crystal molecules for specific material properties.
Collaborations	Prof. Ayon Bhattacharjee, Department of Physics NIT Meghalaya, Shillong Prof. Przemyslaw Kula, Faculty of Advanced Technologies and Chemistry, Military University of Technology, Warsaw, Poland Dr. Debanjan Bhattacharjee, Department of Physics, Manipal University Jaipur