Title: The title "Electrical and Optical Properties of Molecules: A Comprehensive Theoretical and Computational Investigation" accurately reflects the scope and content of the work. It clearly conveys the focus on both electrical and optical aspects, as well as the theoretical and computational methodologies employed.

Abstract: The abstract provides a concise and informative summary of the key findings and their significance. It highlights the crucial role of molecular polarisability in determining electrical conductance, as well as the quantum mechanical underpinnings of optical transitions. The abstract is well-structured and effectively communicates the main contributions of the work.

Introduction: The introduction sets the stage by emphasising the fundamental importance of understanding molecular electrical and optical properties for emerging technologies. It provides a clear motivation for the study and outlines the central aim of developing a unified theoretical framework. The introduction is well-referenced, drawing on relevant literature to contextualise the work.

Methodology: The methodology section is the strongest aspect of this manuscript. It provides complete and rigorous derivations of all key equations, starting from the foundational Schrödinger equation and progressing through molecular polarisability, electrical conductance, optical transition dipole moments, and computational methods. The explanations are clear, and the physical significance of each equation is well-articulated. The inclusion of illustrative figures (e.g., Figures 1 and 2) enhances the clarity of the presentation.

Results: The results section presents a compelling validation of the polarisability-conductance relationship through experimental data and theoretical fitting. The electronic absorption and fluorescence properties are thoroughly characterised, with insightful connections drawn to the underlying electronic structure. The results are well-supported by data presented in tables and figures.

Discussion: The discussion section explores the implications of the findings for molecular electronics and photonics design. It offers practical insights into strategies for optimising electrical conductance and optical properties based on the established structure-property relationships. The limitations of the current approach are appropriately acknowledged, and exciting future research directions are outlined.

Conclusion: The conclusion effectively summarises the key advances and contributions of the work. It highlights the significance of the polarisability-conductance relationship and the quantitative framework for optical property engineering. The broader impact on next-generation molecular-scale technologies is convincingly articulated.

References: The references are comprehensive and up-to-date, drawing from leading journals in the field. They demonstrate the authors' command of the relevant literature and provide appropriate context for the current work.

Overall Assessment:
This is an outstanding manuscript that makes significant contributions to the field of molecular electronics and photonics. The theoretical framework is rigorously developed, and the computational methodologies are state-of-the-art. The results provide valuable insights into the fundamental relationships between molecular structure and electrical/optical properties, with clear implications for rational design.

The manuscript is well-structured, logically organised, and clearly written. The figures and tables effectively support the narrative and enhance the clarity of the presentation. The work is of high novelty and importance, addressing key challenges in the field and offering practical design principles for next-generation molecular devices.

Recommendation: Accept with minor revisio