



Dr. Junias J. Singh

Assistant Professor
Department of Mathematics
School of Engineering
Dayananda Sagar University, Bengaluru, Karnataka,
India

Research: Chemical Graph Theory, Topological Indices, Graph Entropy, QSAR/QSPR and Predictive Modelling

1. ABOUT

Dr. Junias J Singh has completed his Ph.D. in Mathematics at Vellore Institute of Technology (VIT), Vellore. His research focuses on the topological characterization of molecular networks such as nanosheets, nanotubes, and nanowires using graph theoretical frameworks and topological indices. He applies these techniques within QSAR and QSPR models to predict the physical, chemical, and biological properties of nanostructures. He obtained his M.Sc. in Mathematics from Loyola College, Chennai, and his B.Sc. in Mathematics from St. Joseph's College, Tiruchirappalli. He served as a Teaching cum Research Assistant at VIT. He has published five research papers in SCI and SCIE indexed journals and has presented his work at several international conferences. His academic interests include mathematical modelling, nanomaterials, and the integration of graph theory in chemical and materials research.

2. RESEARCH INTERESTS

- Chemical graph theory
- Molecular descriptors
- Topological characterization of complex molecular structures
- Predictive model using QSAR/QSPR techniques

3. ACADEMIC QUALIFICATIONS

- Ph.D. in Mathematics, VIT University, Vellore; 2026
- M.Sc. — Mathematics — Loyola College, Chennai; 2018
- B.Sc. — Mathematics — St. Joseph's College, Tiruchirappalli; 2018

4. PROFESSIONAL EXPERIENCE

- **Assistant Professor** — Department of Mathematics, School of Engineering, Dayananda Sagar University, Bengaluru (November 2025 – Present)
- **Teaching cum Research Assistant (TRA)** — VIT University, Vellore (October 2021 – 2025)

5. RESEARCH HIGHLIGHTS

- **Publications:** Peer-reviewed research publications in SCI/SCIE-indexed journals on graph-theoretic descriptors, entropy measures and predictive modelling of nanomaterials.
- **Awards / Recognitions:** Raman Research Award recognitions at VIT University for research publications (2023–2024).
- **Academic / Conference Roles:** Teaching and academic contributions in mathematics, probability, statistics and quantitative methods.

6. SELECTED PUBLICATIONS

1. J. Singh Junias, Joseph Clement, M.P. Rahul, Micheal Arockiaraj, Krishnan Balasubramanian, Distance-based network topologies of corographenes, Chemical Papers, Vol. 79, No. 12, pp. 8863–8880, 2025
2. M.P. Rahul, Joseph Clement, J. Singh Junias, Micheal Arockiaraj, Krishnan Balasubramanian, Degree-based entropies of graphene, graphyne and graphdiyne using Shannon's approach, Journal of Molecular Structure, Vol. 1260, pp. 132797, 2022
3. J. Singh Junias, Joseph Clement, Weighted bond-additive descriptors of titanium oxide nanosheet, The European Physical Journal Special Topics, Springer, Vol. 233, pp. 2325–2334, 2023
4. J. Singh Junias, Joseph Clement, Predictive analytics of conductance and HOMO LUMO gaps with topological descriptors of porphyrin nanosheets, Physica Scripta, Vol. 99, No. 1, pp. 015208, 2023
5. J. Singh Junias, Joseph Clement, M.P. Rahul, Micheal Arockiaraj, Two-dimensional phthalocyanine frameworks: Topological descriptors, predictive models for physical properties and comparative analysis of entropies with different computational methods, Computational Materials Science, Vol. 235, pp. 112844, 2024

7. ACADEMIC PROFILES

- Google Scholar: [Junias Jaya Singh - Google Scholar](#)
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- Scopus: [57495505900](#)
- ResearchGate: [Junias J Singh](#)

8. CONTACT

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