



Bharathiar University

State University | "A++" Grade by NAAC | 46th Rank in MoE-NIRF
Maruthamalai Road, Coimbatore, Tamil Nadu - 641 046.

Dr K. SENTHILKUMAR Professor Department of Physics Bharathiar University Coimbatore, 641046 Tamil Nadu, India E-mail: ksenthil@buc.edu.in Phone: 9486411335 Office Number: 04222428448	
Research Area <ul style="list-style-type: none">• Molecular Quantum Mechanics• Computational Material Science• Structure Property Relationship	Courses Teaching <ul style="list-style-type: none">• Thermodynamics and statistical mechanics• Quantum mechanics• Numerical Methods• Computer programming with ForTran and Python• Molecular Quantum Mechanics
Research Experience: 23	Teaching Experience: 19
Research Credentials (as on February 2026 – Source: Google scholar) H-index: 31 Citations: 4375 i10-index: 87	
Patents : Granted: 1	
Publications International Journals: 143 National Journals: 1 Books/Chapters: 3 Conferences: 11	
Career At Bharathiar University <ol style="list-style-type: none">1. Designation : Professor Period : January 2021 - Till Date2. Designation : Associate Professor Period : January 2018 - January 20213. Designation : Assistant Professor Period : January 2008 - January 2018 Other Institutes <ol style="list-style-type: none">1. Designation : Lecturer Institution Name : N. G. M. College, Pollachi Period : September 2006 - January 20082. Designation : Post Doctoral Fellow Institution Name : Bristol University, United Kingdom Period : August 2005 - August 20063. Designation : Post Doctoral Fellow Institution Name : Delft University of Technology, The Netherlands Period : August 2002 - June 2005	
Education Ph. D. Subject : Physics Institution : Bharathiar University, Coimbatore - 641 046 Affiliated University : Bharathiar University, Coimbatore - 641 046 Year of Award : June 2002	



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Dr K. SENTHILKUMAR , Professor , Department of Physics

M. Phil.

Subject : Physics

Institution : Bharathiar University, Coimbatore - 641 046

Affiliated University : Bharathiar University, Coimbatore - 641 046

Year of Award : May 1999

M. Sc.

Subject : Physics

Institution : Nallamuthu Gounder Mahalingam College, Pollachi - 642 001

Affiliated University : Bharathiar University, Coimbatore - 641 046

Year of Award : May 1997

B. Sc.

Subject : Physics

Institution : Nallamuthu Gounder Mahalingam College, Pollachi - 642 001

Affiliated University : Bharathiar University, Coimbatore - 641 046

Year of Award : May 1995

Projects

National Level

Ongoing - completed - 5

Research Guidance

Completed

Ph.D. - 13 M.Phil. - 19 PG - 43

On Going

Ph.D. - 2

Institutional Responsibilities

Coordinator - Centre for internet and website services

Period :Sep 2011 - Jul 2025

Nature of Responsibility :Taking care of University LAN, Internet, and website

Nodal Officer

Period :Jun 2022 to Till date

Nature of Responsibility :UGC - Students Grievance

Visits

1. Visiting Scientist at Beijing computational science research center, Beijing, China (2017-06-10 - 2017-06-17)
2. International Congress on Quantum Chemistry 2009 at University of Helsinki, Finland (2009-06-22 - 2009-06-27)
3. Post Doctoral Research Associate at Bristol University, United Kingdom (2005-08-01 - 2006-08-01)
4. Group Symposium on Molecular simulation at Molecular Biophysics, IWR, University of Heidelberg, Heidelberg, Germany (2008-03-21 - 2008-03-21)
5. Sixth international symposium on functional Pi- electron systems at Cornell University, Ithaca, New York, USA (2004-06-13 - 2004-06-18)
6. European Summer School in Quantum Chemistry at Tjornarp Conference Centre, Tjornarp Org. by Department of Theoretical Chemistry, University of Lund, Sweden (2003-08-17 - 2003-08-30)
7. Post Doctoral Researcher at Delft University of Technology, The Netherlands (2002-08-01 - 2005-06-01)
8. Spring college in Numerical methods in electronic structure theory at the Abdus Salam International Center for Theoretical Physics (ICTP), Trieste, Italy (2001-05-07 - 2001-05-25)

Collaborations

1. Dr. R. Karvembu, Professor, Department of Chemistry, National Institute of Technology, Trichy-620 015
2. Dr. D. Nataraj, Professor, Department of Physics, Bharathiar University, Coimbatore- 641046
3. Dr. Daniel Thangadurai, Professor, Department of Chemistry, KPR Institute of Engineering and Technology, Coimbatore -641 407



4. Dr. L. Sandhiya, Scientist, CSIR-National Institute of Science Communication and Policy Research, New Delhi 110012.

Programs organized

1. DST-SERB supported online workshop on electronic structure calculations for molecules and materials (2023-04-17 - 2023-04-24)
2. DST-PURSE supported satellite symposium on physical sciences (2022-09-13 - 2022-09-15)
3. Refresher course in physics (2014-12-03 - 2014-12-23)
4. Workshop on theoretical physics (2013-12-09 - 2013-12-12)
5. Workshop on theoretical physics (2012-12-17 - 2012-12-20)
6. Workshop on theoretical physics (2011-12-19 - 2012-12-22)

Patents

Granted - 1

1. Method to produce graphene quantum dot sheet and its applications 05-2022 397923 Dr. D. Nataraj, Dr. G. Bharathi, Dr. K. Senthilkumar

Selected Publications

1. Unraveling the Autoxidation Mechanisms of Limonene, α -Pinene, and β -Pinene: A Computational Study with Reactivity Prediction Models

The Journal of Physical Chemistry A 10609-10619 (December 2024)
A Bhavadharini, L Sandhiya, K Senthilkumar

2. Hydrogen storage property of the Sc decorated aza-triphenylene based covalent organic framework

Journal of Power Sources Volume 604,234505 (June 2024)
V. M. Vasanthakannan, K Senthilkumar

3. First principle studies on triphenylene-hexathiol-based metal-organic framework for hydrogen storage application

Journal of Energy Storage, 78, 110077 (February 2024)
V.M. Vasanthakannan, M. Pavithrakumar, K. Senthilkumar

4. Tailoring the mechanistic pathways and kinetics of OH-addition reaction of sulfoxaflo and its ecotoxicity assessment

Environmental Science and Pollution Research, 30(17), 50209-50224 (February 2023)
G Manonmani, L Sandhiya, K Senthilkumar

5. Nitrogen- and Boron-Doped Polycyclic Aromatic Hydrocarbons as Hole Transporting Materials for Perovskite Solar Cells

Journal of Electronic Materials, 52, 1461–1473 (December 2022)
M. Pavithrakumar and K. Senthilkumar

6. Modified Fullerenes as an Acceptor in Bulk Heterojunction Organic Solar Cell – A Theoretical study

Physical Chemistry Chemical Physics, 2021, 23, 27468 - 27476 (November 2021)
S. Krishnan and K. Senthilkumar

7. Unimolecular Decomposition of Acetyl Peroxy Radical: A Potential Source for Tropospheric Ketene

Physical Chemistry and Chemical Physics 22. 26819-26827 (November 2020)
L. Sandhiya and K. Senthilkumar



8. Effect of structural fluctuations on charge carrier dynamics in triazene based octupolar molecules

Journal of Physical Chemistry C 118, 27754-27762 (November 2014)
K. Navamani and K. Senthilkumar

9. Analysis of polarization in QM/MM modelling of biologically relevant hydrogen bonds

Journal of the Royal Society Interface 5, S207 (September 2008)
K. Senthilkumar, J.I. Mujika, K. E. Ranaghan, F. R. Manby, A. J. Mulholland and J.N. Harvey

10. Absolute rates of hole transfer in DNA [HOT PAPER, ISI]

Journal of American Chemical Society 127, 14894-14903 (September 2005)
K. Senthilkumar, F.C. Grozema, C.F. Guerra, F.M. Bickelhaupt, F. D. Lewis, Y. A. Berlin, M. A. Ratner and L.D.A. Siebbeles.