




# Bharathiar University

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

<b>Dr K. SENTHILKUMAR</b> Professor Department of Physics Bharathiar University Coimbatore, 641046 Tamil Nadu, India <b>E-mail:</b> ksenthil@buc.edu.in <b>Phone:</b> 9486411335 <b>Office Number:</b> 04222428448	
<b>Research Area</b> <ul style="list-style-type: none"><li>• Molecular Quantum Mechanics</li><li>• Computational Material Science</li><li>• Structure Property Relationship</li></ul>	<b>Courses Teaching</b> <ul style="list-style-type: none"><li>• Thermodynamics and statistical mechanics</li><li>• Quantum mechanics</li><li>• Numerical Methods</li><li>• Computer programming with ForTran and Python</li><li>• Molecular Quantum Mechanics</li></ul>
<b>Research Experience:</b> 23	<b>Teaching Experience:</b> 19
<b>Research Credentials</b> (as on February 2026 – Source: Google scholar) H-index: 31                      Citations: 4375                      i10-index: 87	
<b>Patents :</b> Granted: 1	
<b>Publications</b> International Journals: 143                      National Journals: 1                      Books/Chapters: 3 Conferences: 11	
<b>Career</b> <b>At Bharathiar University</b> <ol style="list-style-type: none"><li><b>1. Designation : Professor</b> Period : January 2021 - Till Date</li><li><b>2. Designation : Associate Professor</b> Period : January 2018 - January 2021</li><li><b>3. Designation : Assistant Professor</b> Period : January 2008 - January 2018</li></ol> <b>Other Institutes</b> <ol style="list-style-type: none"><li><b>1. Designation : Lecturer</b> Institution Name : N. G. M. College, Pollachi Period : September 2006 - January 2008</li><li><b>2. Designation : Post Doctoral Fellow</b> Institution Name : Bristol University, United Kingdom Period : August 2005 - August 2006</li><li><b>3. Designation : Post Doctoral Fellow</b> Institution Name : Delft University of Technology, The Netherlands Period : August 2002 - June 2005</li></ol>	
<b>Education</b> <b>Ph. D.</b> 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, $\alpha$ -Pinene, and $\beta$ -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.