




Bharathiar University

State University I "A++" Grade by NAAC I 21st Rank in MoE-NIRF
Maruthamalai Road, Coimbatore, Tamil Nadu - 641 046.

<p>Dr K. SENTHILKUMAR Professor Department of Physics</p> <p>Bharathiar University Coimbatore, 641046 Tamil Nadu, India</p> <p>E-mail: ksenthil@buc.edu.in phone: 9486411335</p>	
<p>Research Area Molecular Quantum Mechanics, Computational Material Science, Structure Property Relationship</p>	<p>Courses Teaching Thermodynamics and statistical mechanics, Quantum mechanics, Numerical Methods, Computer programming with ForTran and Python</p>
<p>Research Experience: 21</p>	<p>Teaching Experience: 17</p>
<p>Research Credentials (as on October 2023 – Source: Google scholar) H-index: 25 Citations: 3420 i10-index: 72</p>	
<p>Publications International: 125 National: 1 Conferences: 5</p>	
<p>Career (At BU) Assistant Professor(January 2008 - January 2018) Associate professor(January 2018 - January 2021) Professor (January 2021 -) (Other Institutes) Lecturer(September 2006 - January 2008) Post Doctoral Fellow(August 2005 - August 2006) Post Doctoral Fellow(August 2002 - June 2005)</p>	
<p>Education Ph. D. - Physics, Bharathiar University, Coimbatore - 641 046, June 2002 M. Phil. - Physics, Bharathiar University, Coimbatore - 641 046, May 1999 M. Sc. - Physics, Nallamuthu Gounder Mahalingam College, Pollachi - 642 001, May 1997 B. Sc. - Physics, Nallamuthu Gounder Mahalingam College, Pollachi - 642 001, May 1995</p>	
<p>Projects National Level Ongoing - 2 completed - 3</p>	<p>Research Guidance Completed Ph.D. - 11 M.Phil. - 19 PG - 36 On Going Ph.D. - 4 PG - 3</p>
<p>Institutional Responsibilities Coordinator - University Data Center & Internet - Taking care of LAN & Internet Facility of Entire University</p>	



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Dr K. SENTHILKUMAR , Professor , Department of Physics

Visits

1. Visiting Scientist at Beijing computational science research center, Beijing, China(2017-06-10)
2. International Congress on Quantum Chemistry 2009 at University of Helsinki, Finland(2009-06-22)
3. Post Doctoral Research Associate at Bristol University, United Kingdom(2005-08-01)
4. Group Symposium on Molecular simulation at Molecular Biophysics, IWR, University of Heidelberg, Heidelberg, Germany(2008-03-21)
5. Sixth international symposium on functional Pi- electron systems at Cornell University, Ithaca, New York, USA(2004-06-13)
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)
7. Post Doctoral Researcher at Delft University of Technology, The Netherlands(2002-08-01)
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)

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.

Selected Publications

International - 5

1. A Computational Perspective on the Chemical Reaction of HFO-1234zc with the OH Radical in the Gas Phase and in the Presence of Mineral Dust (G. Manonmani, L. Sandhiya, and K. Senthilkumar) - December 2022
2. Unimolecular Decomposition of Acetyl Peroxy Radical: A Potential Source for Tropospheric Ketene (L. Sandhiya and K. Senthilkumar) - November 2020
3. Effect of structural fluctuations on charge carrier dynamics in triazene based octupolar molecules (K. Navamani and K. Senthilkumar) - November 2014
4. Analysis of polarization in QM/MM modelling of biologically relevant hydrogen bonds (K. Senthilkumar, J.I. Mujika, K. E. Ranaghan, F. R. Manby, A. J. Mulholland and J.N. Harvey) - September 2008
5. Absolute rates of hole transfer in DNA [HOT PAPER, ISI] (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.) - September 2005