

Faculty Profile of Dr.K.Senthilkumar



Dr.K.Senthilkumar
Professor
Department of Physics

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Phone No:0422-2428448

Mobile No:9486411335

Research Area

- Molecular Quantum Mechanics
- Computational Material Science
- Structure Property Relationship

Education & Career

Education

Ph. D.

Subject : Physics

Institution : Bharathiar University

Affiliated University : Bharathiar University

Year of Award : 2002

M. Phil.

Subject : Physics

Institution : Bharathiar University

Affiliated University : Bharathiar University

Year of Award : 1999

M. Sc.,

Subject: Physics

Institution : Nallamuthu Gounder Mahalingam College, Pollachi - 642 001

Affiliated University : Bharathiar University

Year of Award : 1997

B. Sc.,

Subject: Physics

Institution: Nallamuthu Gounder Mahalingam College, Pollachi - 642 001

Affiliated University: Bharathiar University

Year of Award: 1995

Career**At Bharathiar University****3. Professor (15.01.2021 to Till date)**

Department of Physics

2. Associate Professor (15.01.2018 to 14.01.2021)

Department of Physics

1. Assistant Professor (14.01.2008 to 14.01.2018)

Department of Physics

Past Experience**3. Lecturer in Physics (From September, 2006 to January, 2008)**

Nallamuthu Gounder Mahalingam College,

Pollachi - 642 001

2. Post Doctoral Research Associate (From August, 2005 to August, 2006)

Bristol University
United Kingdom

1. Post Doctoral Researcher (From August, 2002 to June, 2005)

Delft University of Technology
The Netherlands

Awards

1. Young Scientist award awarded by DST, India in 2009
2. Post Doctoral Research Assistant at Bristol University, United kingdom in 2005
3. Post Doctoral Researcher at Delft University of Technology, The Netherlands in 2002
4. Senior Research Fellowship awarded by CSIR, India in 2000

Membership

Professional Bodies

Member

Member: American Chemical Society - USA
Year: 2015

Editorial Board member

Journal: Computational Theoretical Chemistry Journal (Elsevier)

Visits

Country Visited : China

Duration of Visit : 10th to 17th June 2017

Purpose of Visit : Visiting Scientist at Beijing computational science research center, Beijing.

Country Visited : Finland

Duration of Visit : 22 nd to 27th June 2009

Purpose of Visit : International Congress on Quantum Chemistry 2009
at University of Helsinki

Country Visited : United Kingdom

Duration of Visit : August 2005 – August 2006

Purpose of Visit : Post Doctoral Research Associate at Bristol University

Country Visited : Germany

Duration of Visit : 21 st March 2005

Purpose of Visit : Group Symposium on Molecular simulation at Molecular
Biophysics, IWR, University of Heidelberg, Heidelberg

Country Visited : USA

Duration of Visit : 13 th to 18 th June 2004

Purpose of Visit : Sixth international symposium on functional Pi- electron
systems at Cornell University, Ithaca, New York

Country Visited : Sweden

Duration of Visit : 17 th to 30 th August 2003

Purpose of Visit : European Summer School in Quantum Chemistry
at Tjornarp Conference Centre, Tjornarp Org. by Department of Theoretical
Chemistry, University of Lund

Country Visited : The Netherlands

Duration of Visit : August 2002 to June 2005

Purpose of Visit : Post Doctoral Researcher at Delft University of
Technology, The Netherlands

Country Visited : Italy

Duration of Visit : 7 th to 25 th May 2001

Purpose of Visit : Spring college in Numerical methods in electronic
structure theory at the Abdus Salam International Center for Theoretical
Physics (ICTP), Trieste

Collaborators

[Dr. R. Karvembu](#)

Professor

Department of Chemistry

National Institute of Technology

Trichy-620 015, India

Dr. D. Nataraj

Professor

Department of Physics

Bharathiar University

Coimbatore- 641046.

Dr. T. Daniel Thangadurai

Head of the Department

M.Tech Nanoscience and Technology

Sri Ramakrishna Engineering College

Vattamalaipalayam, N.G.G.O Colony P.O,

Coimbatore - 641 022

Others

Projects

Funded Projects(National Level)

- [Ongoing - 02](#)
- [Completed - 03](#)

1. UGC, India

Title of the project: Quantum mechanical and molecular mechanical studies on the reactions of pollutants in atmosphere and in water

Funding Agency: UGC, India

Amount: Rs. 13,43,800

Duration: 2012-2015

2. DRDO, India

Title of the project: Theoretical studies on charge transport properties in organic field effect transistor

Funding Agency: DRDO, India

Amount: Rs. 7,40,100

Duration: 2010-2012

3. DST, India

Title of the project: Effect of structural fluctuations and environment on charge transport in π -stacked and conjugated organic molecules

Funding Agency: DST, India

Amount: Rs. 17,87,200

Duration: 2010-2012

1. TANSCH, Tamil nadu

Title of the project : Probing the mechanism, thermochemistry and kinetics of the degradation of organic air pollutants in the atmosphere

Funding Agency : TANSCH, Tamil nadu

Amount : Rs. 21.33 Lakhs

Duration : 2021-2024

2. DST-SERB, India

Title of the project: Driving perovskite photovoltaics towards next generation solar cells through computational material engineering

Funding Agency: DST-SERB, India

Amount: Rs. 22,69,764

Duration: 2020-2023

Department Level Projects

Consultancy Projects

- [Ongoing](#)
 - [Completed](#)
-

Research Guidance

- [Post Doc.](#)
- [Ph.D.](#)
- [M.Phil.](#)
- [M.Sc.](#)

Ongoing

Completed

Ongoing-04

Ms. S. V. Thoshiba

Filed of research: Theoretical studies on the mechanism, thermochemistry and kinetics of the atmospheric chemical reactions

Date of Registration: 01.11.2022

Ms. A. Bhavadharini

Filed of research: Probing the mechanism, thermochemistry and kinetics of the degradation of organic air pollutants in the atmosphere

Date of Registration: 01.11.2022

Mr. V. M. Vasanthakannan

Field of research: Electronic structure calculations for molecules and materials

Date of Registration: 01.12.2021

Mr. M. Pavithrakumar

Field of research: Charge transport and opto-electronics properties of organic semiconductor materials

Date of Registration: 01.10.2019

Completed-11

Dr. G. Manonmani

Title of the thesis: Probing the Mechanism, Kinetics, and Toxicity of the Degradation of Air Pollutants in the Atmosphere

year of award: 2022

Dr. S. Krishnan

Title of the thesis: Electronic structure investigations on materials for new generation photovoltaic applications

year of award: 2022

Dr. M. Vinodha

Title of the thesis: Structure and Electronic Properties of Organic Molecules and Molecule/Metal interfaces

Year of award: 2021

Dr. R. Bhuvaneswari

Title of the thesis: Computational perspective on the atmospheric oxidation of few volatile organic compounds initiated by hydroxyl radical

Year of award: 2020

Dr. M. Gnanaprakasam

Title of the thesis: Theoretical investigation on mechanism and kinetics of the atmospheric chemical reactions of few volatile organic compounds

Year of award: 2018

Dr. M. Sowmiya

Title of the thesis: Theoretical studies on the interaction of molecules with anatase TiO₂ (001) surface for medical, catalytic and dye-sensitized solar cell applications

Year of award: 2017

Dr. S. Ponnusamy

Title of the thesis: Theoretical studies on the reaction mechanism and kinetics of atmospheric pollutants with hydroxyl radical

Year of award: 2017

Dr. K. Navamani

Title of the thesis: Charge Carrier Dynamics in Few π -stacked Organic Molecules

Year of award: 2015

Dr. L. Sandhiya

Title of the thesis: Theoretical studies on the mechanism and kinetics of atmospheric chemical reactions

Year of award: 2015

Dr. R. Nithya

Title of the thesis: Quantum chemical studies on the opto-electronic properties π -conjugated organic molecules

Year of award: 2014

Dr. G. Saranya

Title of the thesis: Quantum chemical studies on optical and charge transport properties of organic molecules and organic/metal Interfaces

Year of award: 2014

Ongoing

Completed-19

Ms. Rose Denny

Title of the thesis: Computational Investigation on the Reaction of CH_3CHOO with water molecules

Year of award: 2022

Ms. J. Sheebha Veronica

Title of the thesis: Structure and charge transport properties of bridge mediated charge transfer complex pentacene/benzothiadiazole cocrystal

Year of award: 2022

K. Kanimozhi

Title of the thesis: Effect of stacking angle fluctuation on charge carrier mobility in π -stacked triazole based star-shaped molecules

Year of award: 2018

S. Indhu

Title of the thesis: Theoretical study on the reaction mechanism and kinetics

of sulfonylamine with water molecules

Year of award: 2017

M. Rajeswari

Title of the thesis: Opto-electronic and adsorption properties of azobenzene dyes on TiO_2 surface

Year of award: 2016

R. Jayabharathi

Title of the thesis: Theoretical Studies on the Mechanism and Kinetics of the Reaction of Terbacil with OH Radical

Year of award: 2015

N. Saranya

Title of the thesis: Theoretical studies on charge transport properties of 3,5 bis-[2-(3,4,5-trimethoxy -phenyl)-vinyl]-1H-pyrazole

Year of award: 2014

M. Gnanaprakasam

Title of the thesis: Mechanism and Kinetics of the Atmospheric oxidation of Naphthalene initiated by OH radical

Year of award: 2013

M. Sowmiya

Title of the thesis: Structural, optical and charge transport properties of cyclopentadithiophene derivatives: A theoretical study

Year of award: 2012

S. Ponnusamy

Title of the thesis: Studies on the mechanism, kinetics and global warming potential of the atmospheric degradation of perfluoropolymethylisopropyl ether by OH radical

Year of award: 2012

R. Deepika

Title of the thesis: Adsorption of pentacene on Pd(100) surface: structural and electronic properties from first principle study

Year of award: 2012

C. Kalaiarasi

Title of the thesis: Theoretical studies on charge transport properties on

Ph4DP and Ph4DTP molecules

Year of award: 2012

S. Yuvarani

Title of the thesis: A theoretical study of structural and electronic properties of pentacene/Al(100) interface

Year of award: 2011

M. Vennila

Title of the thesis: Theoretical studies on the reaction mechanism of sulfadoxine with pi-acceptors

Year of award: 2011

G. Vasugi

Title of the thesis: Absorption and Emission properties of Borondipyrromethene dye and its substituted analogs

Year of award: 2010

A. Shanmugavani

Title of the thesis: Quantum chemical studies on structure and conformational stability of D-Sorbitol and D-Sorbitol-8H₂O complexes

Year of award: 2010

N. Lakshmi

Title of the thesis: Atmospheric reaction pathways and kinetics of the reaction of 1,4-thioxane with OH radical

Year of award: 2010

G. Saranya

Title of the thesis: Studies on charge transport in π -stacked liquid crystalline molecules THDP and THDDP.

Year of award: 2009

R. Nithya

Title of the thesis: Structural and spectral properties of 4-Bromo-1-naphthyl chalcones-A quantum chemical study.

Year of award: 2009

Completed-39

K. Hari Prahadhis

Title of the thesis: Understanding the Proton Transfer from Pentazole (N₅H) to Water Cluster: A Theoretical Study

Year of award: 2024

M. Rishi Narayani

Title of the thesis: Understanding the Ozonolysis Reaction of Alkenes Containing Nitro and Amino groups - A Computational Study

Year of award: 2024

N. J. Swetha

Title of the thesis: A Theoretical Investigation on the Adsorption of Graphene on Brucite and Al-doped Brucite surfaces

Year of award: 2024

N. Santhana Raj

Title of the thesis: Theoretical studies on the electron capturing property of fluoro cubane derivatives

Year of award: 2023

M. Valarmathi

Title of the thesis: Theoretical study on the mechanism and thermochemistry of criegee intermediate CH₂OO with CO in the absence and presence of N₂O catalyst

Year of award: 2023

C. Durgadevi

Title of the thesis: Theoretical studies on the interaction of Formic acid with the abundant gas molecules in the atmosphere (CO₂, H₂O, N₂, N₂O)

Year of award: 2023

M. Diya

Title of the thesis : Theoretical study on the mechanism and thermochemistry of OH radical initiated oxidation reaction of HNCO

Year of award: 2022

K. Sharmila

Title of the thesis : Theoretical study on the mechanism and thermochemistry of reaction of HNCO with CH₃, H, Cl and CN radicals

Year of award: 2022

A. Bhavadharini

Title of the thesis : Synthesis and characterization of NaLiLaTiO₂ solid electrolyte for electrochemical storage devices

Year of award: 2022

N. Anusree Surendran

Title of the thesis: Studying the interactions of metal ions with nucleobases through the density of states analysis

Year of award: 2021

C. Sandhiya

Title of the thesis: theoretical study on the mechanism and thermochemistry of OH-initiated reaction of HFO-1234ZC

Year of award: 2021

M. Muthu

Title of the thesis: Quantum mechanical and molecular mechanics study on the stacking of 1,3,5-Triphenyltriazine

Year of award: 2021

M. Sankari

Title of the thesis: Dibenzocoronene tetracarboxdiimide derivative using Molecular Mechanics and Molecular Dynamics Simulations.

Year of award: 2020

V. Sandhiyadevi

Title of the thesis: Sulfolysis of Criegee intermediates (CIs): A potential route for the production of H₂SO₃

Year of award: 2019

I. Ajin

Title of the thesis: Effect of structural fluctuation on charge transport in π -stacked triphenylene derivatives - a theoretical study

Year of award: 2019

S.P. Keerthana

Title of the thesis: A density functional theory investigation on the reaction mechanism and thermochemistry of isoprene epoxydiols formation in the atmosphere

Year of award: 2019

K. Nandhakumar

Title of the thesis: Theoretical study on stacking angle fluctuations in TriB (Triphenyl Benzene) derivative using molecular dynamics simulation

Year of award: 2019

S. Ram Prakash

Title of the thesis: Effect of Stacking angle fluctuation on charge carrier mobility in pi- stacked Tris (N- Phenyltriazole)- A DFT Study

Year of award: 2018

U. Abdul Kareem

Title of the thesis: Molecular mechanics and molecular dynamics study on stacking distance and stacking angle in tris(n- Phenyltriazole) derivative

Year of award: 2018

T. Kiruthika

Title of the thesis: Theoretical study on Gas phase reaction of methyl chavicol with NO₃ radical

Year of award: 2018

K. Subramanyan

Title of the thesis: Computational insight into impact of stacking angle on charge transport in π

Year of award: 2017

T.P. Praseeda

Title of the thesis: Theoretical studies on the degradation mechanism of diuron through the reaction with OH radical

Year of award: 2017

J. Evangelin Princy

Title of the thesis: Structure, Interaction and adsorption spectra of fused imidazolium cation with BF₄⁻, CF₃SO₃⁻ anions

Year of award: 2016

G. Manonmani

Title of the thesis: Theoretical studies on the reaction of criegee intermediates CH_2OO and CH_3CHOO with water dimer

Year of award: 2016

N. Priya

Title of the thesis: Theoretical studies on interaction between stacked guanine-cytosine base pairs

Year of award: 2015

S. Bagyalakshmi

Title of the thesis: Adsorption of Tetracyanoquinodimethane and Tetrathiafulvalene on Al (100) surface: A First Principle Study

Year of award: 2015

S. Malarvizhi

Title of the thesis: Structural and Energetical Properties of 1-acyl-3-substituted Thiourea Isomers

Year of award: 2014

M. Rajeswari

Title of the thesis: A theoretical Study on the Structure and Stability of 3,5-bis-[2-(3,4,5-trimethyl-phenyl-vinyl)]-1H-Pyrazole and its dimer

Year of award: 2014

R. Sahana banu

Title of the thesis: Mechanism and Kinetics of the Nitration of Tyrosine by O_3 and NO_2

Year of award: 2013

J. Shoba

Title of the thesis: Adsorption of Perfluoropentacene on Al (100) Surface – A theoretical Study

Year of award: 2013

N. Vanitha Lakshmi

Title of the thesis: A Theoretical investigation on Adsorption of Pentacene on SiO_2 (100) Surface

Year of award: 2012

K. Mahalaksmi

Title of the thesis: Reaction Mechanism and Kinetics of the Oxidation of NO₂ by O₃ in the Atmosphere – Theoretical Study

Year of award: 2012

B. Sathyamoorthy

Title of the thesis: Theoretical studies on the atmospheric reactions of 2,3-dimethylphenol with OH radical

Year of award: 2011

C. Kalaiarasi

Title of the thesis: A theoretical study on structural and energetical properties of (CrO₃)_n (n=1-5) and (TiO₂)_n (n=1-4) clusters

Year of award: 2011

M. Vennila

Title of the thesis: Study of stacking angle in discotic liquid crystalline molecules THDP and THDDP using molecular dynamic simulations.

Year of award: 2010

S. Yuvarani

Title of the thesis: Potential energy surface characterization of HCCO+NO₂ reaction

Year of award: 2010

L. Sandhiya

Title of the thesis: Theoretical studies on dimers of barbituric acid.

Year of award: 2009

M. Kousalya

Title of the thesis: Density functional studies on structure, stability and optical absorption of unsubstituted and substituted 4-bromo-1-naphthyl chalcones.

Year of award: 2009

G. Vasugi

Title of the thesis: Effect of substitution and conformation on the stability of 4-bromo-1-naphthyl chalcones.

Year of award: 2009

Research Publication

- [International](#)
- [National](#)
- [Patents](#)
- [Conferences](#)
- [Books/Chapters](#)
- [Database](#)

Reverse Chronological Order

2022-2024

126. [Triselenasumanene-based organic molecules as donor and hole-transporting materials for next-generation solar cells](#)

M. Pavithrakumar and K. Senthilkumar

Journal of Physics and Chemistry of Solids, 190, 111961 (2024)

125. [First principle studies on triphenylene-hexathiol-based metal-organic framework for hydrogen storage application](#)

V.M. Vasanthakannan, M. Pavithrakumar, K. Senthilkumar

Journal of Energy Storage, 78, 110077 (2024)

124. [Theoretical investigations of the substituent effect on the opto-electronic properties of the linearly fused naphthadithiophene-based molecules](#)

Jothi Balakrishnan, Pavithrakumar Muthukumar, David Stephen Arputharaj, Pitchumani Violet Mary Christopher, Selvaraju Karuppannan, Senthilkumar Kittusamy

The Journal of Computational Chemistry, 1 (2024).

123. [Reaction of Criegee Intermediates with SO₂—A Possible Route for Sulfurous Acid Formation in the Atmosphere](#)

Gunasekaran Manonmani, Lakshmanan Sandhiya, Kittusamy Senthilkumar
ACS Earth and Space Chemistry, 7, 10, 1890–1904 (2023)

122. [Tailoring the mechanistic pathways and kinetics of the OH-addition reaction of sulfoxaflo and its ecotoxicity assessment](#)

Gunasekaran Manonmani, Lakshmanan Sandhiya, Kittusamy Senthilkumar
Environmental Science and Pollution Research, 30, 50209–50224 (2023)

121. [The association of air quality and complex atmospheric oxidation chemistry in the dispersion and deposition of SARS-CoV-2-laden aerosols](#)
Sandhiya Lakshmanan, Ranjana Aggarwal, Kittusamy Senthilkumar,
Anupama Upadhyay
Environmental Science: Advances, 2, 11, 1540-1553 (2023)
120. [New insights into pertinent Fe-complexes for the synthesis of iron via the instant polyol process](#)
Sivaranjani Kottaipalayam Somasundaram, Ana Guilherme Buzanich,
Franziska Emmerling, Sangameswaran Krishnan, Kittusamy Senthilkumar,
Raphael Justin Joseyphus
Physical Chemistry Chemical Physics, 25, 21970-21980 (2023)
119. [Nitrogen- and Boron-Doped Polycyclic Aromatic Hydrocarbons as Hole Transporting Materials for Perovskite Solar Cells](#)
M. Pavithrakumar and K. Senthilkumar
Journal of Electronic Materials, 52, 1461–1473 (2023)
118. [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
J. Phys. Chem. A 126, 51, 9564–9576 (2022)
117. [Tetrathiafulvalene Derivatives as Hole-Transporting Materials in Perovskite Solar Cell](#)
S Krishnan, K Senthilkumar
The Journal of Physical Chemistry A, 126, 31, 5079–5088 (2022)
116. [Opto-Electronic Properties of Quasi-Planar Boron clusters-A DFT Investigation](#)
S Krishnan, K Senthilkumar
Chemical Physics Letters, 139914 (2022)
115. [Coordination Behavior of Acylthiourea Ligands in Their Ru \(II\)-Benzene Complexes– Structures and Anticancer Activity](#)
Srividya Swaminathan, Jebiti Haribabu, Mohamed Kasim Mohamed
Subarkhan, Gunasekaran Manonmani, Kittusamy Senthilkumar, Nithya
Balakrishnan, Nattamai Bhuvanesh, Cesar Echeverria, Ramasamy Karvembu
Organometallics, 41, 13, 1621-1630 (2022)

114. [Mechanism, kinetics and Ecotoxicity Assesment of OH- initiated oxidation reactions of sulfoxaflo](#)

G. Manonmani, L. Sandhiya and K. Senthilkumar

Journal of Physical Chemistry A 125, 46, 10052-10064, (2021)

113. [Modified Fullerenes as an Acceptor in Bulk Heterojunction Organic Solar Cell – A Theoretical study](#)

S. Krishnan and K. Senthilkumar

Physical Chemistry Chemical Physics, 2021, 23, 27468 - 27476

112. [A Comparative investigation on the scavenging of 2, 2-diphenyl-1-picrylhydrazyl radical by the natural antioxidants \(+\) catechin and \(-\) epicatechin](#)

S Anitha, S Krishnan, K Senthilkumar, V Sasirekha

Journal of Molecular Structure, 1242, 130805, (2021)

111. [Charge Transport and Optical Absorption Properties of Dibenzocoronene Tetracarboxdiimide Based Liquid Crystalline Molecules A Theoretical Study](#)

M. Pavithrakumar, S. Krishnan and K. Senthilkumar

Journal of Physical ChemistryA 125, 3852-3862, (2021)

110. [Investigation on Surface interaction between Graphene Nanobuds and Cerium\(III\) via Fluorescence excimer, Theoretical, Real water sample, and Bioimaging studies](#)

V.R.Pavithra, T. D. Thangadurai, G. Manonmani, K. Senthilkumar, D. Nataraj, J.Jiya, K. Nandakumar and S. Thomas

Materials Chemistry and Physics 264, 124453, (2021)

109. [Room temperature weakly ferromagnetic energy band opened graphene quantum dot coupled solid sheets - A possible carbon based dilute magnetic semiconductor](#)

G. Bharathi, D. Nataraj, O. Y. Khyzhun, D.T. Thangadurai, K. Senthilkumar, M. Sowmiya, R. Kathiresan, P. Kolandaivel,

M. Gupta, D. Phase, N. Patra, S. N. Jha, D. Bhattacharyya

Applied Surface Science 548, 149195, (2021)

108. [Influence of shape and configuration of a sensitizer molecule on the efficiency of DSSC -A Theoretical insight](#)

S. Krishnan and K. Senthilkumar

RSC Advances 11, 5556-5567, (2021)

2020

107. [Unimolecular Decomposition of Acetyl Peroxy Radical: A Potential Source for Tropospheric Ketene](#)

L. Sandhiya and K. Senthilkumar

Physical Chemistry and Chemical Physics 22, 26819-26827, (2020)

106. [Aggregation induced emission behavior in oleylamine acetone system and its application to get improved photocurrent from In₂S₃ quantum dots](#)

S. Ramya, D. Nataraj, S. Krishnan, S. Premkumar, T. Thrupthia, A. Sangeetha, K. Senthilkumar and T. D. Thangadurai

Nature Scientific Reports 10, 19712, (2020)

105. [Adsorption of phenanthroline and its derivatives on Au \(111\) surface – Influence of substitution on structure and electronic properties](#)

M.Vinodha, S.Krishnan, S.Bagyalakshmi and K.Senthilkumar

Computational Materials Science 182, 109778, (2020)

104. [Insight into the Photophysics of Dual Strong Emission \(Blue & Green\) Producing Graphene Quantum Dot Clusters and their Application Towards Selective and Sensitive Detection of Trace Level Fe³⁺ and Cr⁶⁺ Ions](#)

G. Bharathi, D. Nataraj, S. Premkumar, P. Saravanan, D. T. Thangadurai, O. Khyzhun, K. Senthilkumar, P. Kathiresan,, P. Kolandaivel, M. Gupta and D. Phase

RSC Advances 10, 26613-26630, (2020)

103. [Hydrolysis of HNSO₂: A Potential Route for Atmospheric Production of H₂SO₄ and NH₃](#)

G. Manonmani, L. Sandhiya and K. Senthilkumar

International Journal of Quantum Chemistry 120, e26182, (2020)

102. [Theoretical investigation on the structure and antioxidant activity of \(+\) catechin and \(–\) epicatechin – a comparative study](#)

S. Anitha , S. Krishnan , K. Senthilkumar and V. Sasirekha

Molecular Physics, 118, e1745917, (2020)

101. [Mechanism and kinetics of Diuron Oxidation by Hydroxyl Radical Addition Reaction](#)

G. Manonmani, L. Sandhiya and K. Senthilkumar

Environmental Science and Pollution Research 27 (2020) 12080-12095

100. [First Principle Studies on the Atmospheric Oxidation of HFC-C1436 Initiated by OH radical](#)

R. Bhuvaneswari and K. Senthilkumar

New Journal of Chemistry 44, 2070-2082, (2020)

99. [A comprehensive quantum chemical study on the mechanism and kinetics of atmospheric reactions of 3-Chloro-2-methyl-1-propene with OH radical](#)

R. Bhuvaneswari and K. Senthilkumar

Theoretical Chemistry Accounts 139, 2, (2020)

2019-2004

98. [Effect of Site Energy Fluctuation on Charge Transport in Disordered Organic Molecules](#)

K. Navamani, Swapan K. Pati, and K. Senthilkumar

Journal Chemical Physics 151, 224301, (2019)

97. [Mechanism and Kinetics of Diuron Oxidation Initiated by Hydroxyl Radical – Hydrogen and Chlorine Atom Abstraction Reactions](#)

G. Manonmani, L. Sandhiya and K. Senthilkumar

Journal of Physical Chemistry A 123, 8954-8967, (2019)

96. [Atmospheric Oxidation Mechanism and Kinetics of 2-Bromo-4, 6-dinitroaniline by OH radical – A Theoretical Study](#)

M. Gnanaprakasam, G. Saranya, S. Bandaru, N. JOURNAL English and K. Senthilkumar

Physical Chemistry and Chemical Physics 21, 21109-21127, (2019)

95. [Graphene Nanobuds: A New Second-Generation Phosgene Sensor with Ultralow Detection Limit in Aqueous Solution](#)

P.V. Ravi, D. T. Thangadurai, D. Nataraj, K. Senthilkumar, G. Manonmani, N. Kalarikkal, S. Thomas, P. Govindh

ACS Applied Materials & Interfaces 11 (2019) 19339-19349

94. [Theoretical Study on the Gas Phase Reaction of Methyl Chavicol with Hydroxyl Radical](#)

R. Bhuvaneswari and K. Senthilkumar

Computational and Theoretical Chemistry 1151, 78-90, (2019)

93. [Mechanism and Kinetics of the Oxidation of Dimethyl Carbonate by Hydroxyl Radical in the Atmosphere](#)

M. Gnanaprakasam, L. Sandhiya and K. Senthilkumar

Environmental Science and Pollution Research 26, 3357-3367, (2019)

92. [Adsorption of Tetracyanoquinodimethane and Tetrathiafulvalene on Aluminium \(100\) surface - A First Principle Study of Structural and Electronic Properties](#)

M. Vinodha and K. Senthilkumar

Journal of Molecular Simulation 45, 492-500, (2019)

91. [Theoretical Investigation on the Mechanism and Kinetics of Atmospheric Reaction of Methylchloroacetate with Hydroxyl Radical](#)

M. Gnanaprakasam, L. Sandhiya and K. Senthilkumar

Journal of Physical Chemistry A 122. 9316-9325, (2018)

90. [Atmospheric Oxidation Mechanism and Kinetics of Hydrofluoroethers CH₃OCF₃, CH₃OCHF₂ and CHF₂OCH₂CF₃ by OH Radical: A Theoretical Study](#)

S. Ponnusamy, L Sandhiya and K. Senthilkumar

Journal of Physical Chemistry A 122. 4972-4982, (2018)

89. [Theoretical probe on modified organic dyes for high-performance Dye-Sensitized Solar Cell](#)

S. Krishnan and K. Senthilkumar

Current Applied Physics 18, 1071-1079, (2018)

88. [Mechanism and kinetics of the reaction of methyl acetate with Cl atom - A theoretical study](#)

M. Gnanaprakasam, L. Sandhiya and K. Senthilkumar

Computational and Theoretical Chemistry 1131, 40-50, (2018)

87. [Mechanism and Kinetics of the Degradation of Terbacil initiated by OH radical - A Theoretical Study](#)

S. Ponnusamy, L Sandhiya and K. Senthilkumar

Chemical Physics 501, 110-120, (2018)

86. [Counter anion effect on structural, opto-electronic and charge transport properties of fused \$\pi\$ -conjugated imidazolium compound](#)

M. Vinodha and K. Senthilkumar

Molecular Physics 116, 1145-1152, (2017)

85. [Exploring the Mechanisms for the Radical Induced Damage of 6-Thioguanine](#)

L Sandhiya and K. Senthilkumar

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Title of the Invention : Method to produce graphene quantum dot sheet and its applications

Name of the Inventors : Dr. D. Nataraj, Dr. G. Bharathi, Dr. K. Senthilkumar

Department : Department of Physics, Bharathiar University

Patent Number : 397923

Date of Grant : 27.05.2022

Title of the Presentation : A Perspective on Molecular Quantum Mechanics

Event: Summer Training Program in Physics – 2020

Organized by: The Academy of Sciences, Chennai & Dept. of Nanoscience and Technology, Bharathiar University

Date: 24th July 2020

Invited Lecture (online)

Title of the Presentation : An Overview of Molecular Quantum Mechanics and its Application to Model Atmospheric Chemical Reactions

Event: National Symposium on Recent Advances in Chemistry

Organized by: Dept. of Chemistry, Pondicherry University

Date:: 19th February 2020

Invited Lecture

Title of the Presentation : An overview of Molecular Quantum Mechanics and its Applications in Opto-Electronic

Event: State Level Symposium on Spectroscopic Perspective of Quantum Dots

Organized by: Govt. Arts College for Women, Salem

Date: 23rd September 2019

Invited Lecture

Title of the Presentation : Programming with ForTran

Event: National workshop on Programming for data analytics

Organized by: Tamil Nadu Agricultural University, Coimbatore

Date: 1st, 2nd and 5th August 2019

Invited Lecture

Title of the Presentation : Application of DFT to Find and Tune the Suitable Materials for Solar Energy Applications

Organized by: Beijing computational science research center, Beijing, China

Date: 14th June 2017

Title of the Presentation : Physics and Chemistry of Materials through Quantum Mechanics

Event: Quality improvement programme in advances in new engineering materials

Organized by: Coimbatore institute of Technology, Coimbatore

Date: 26 November 2015

Invited Lecture

Title of the Presentation : Invited Lecture Charge Transport Properties of π -Conjugated Oligomers – A Theoretical Study

Event: Symposium on Theoretical and Computational Chemistry - Frontiers and Challenges

Organized by: Bharathidasan University, Tiruchirappalli

Date: 14-15 June 2013

Invited Lecture

Title of the Presentation : Physics and Chemistry of Molecules through Quantum Mechanics

Event: Short term Course in Computational Methods in Chemistry

Organized by: National Institute of Technology, Tiruchirappalli

Date: 23-27 July 2012

Invited Lecture

Title of the Presentation :

1. Optical and conducting properties of fluoranthene and benzo (k) fluoranthene derivatives – A DFT Study
2. Theoretical studies of the oxidative degradation of dimethylphenols by OH radical in the atmosphere

Event: Indian Institute of Technology, Kanpur

Organized by: IICT, Hyderabad

Date:: 2-5 November 2011

Papers presented

Title of the Presentation :

1. A Theoretical Study of Structural and Electronic Properties of Pentacene/Al(100) Interface
2. Theoretical studies on charge transport in thiazolothiazole, thiazole and thiophene based oligomers
3. Theoretical Studies on the atmospheric reaction of 1,4-thioxane with OH, NO₃ and O₃
4. Theoretical Studies on Charge Transport Properties of Tris(N-Saclicylideneanilines)

Event: Theoretical Chemistry Symposium 2010 (TCS10)

Organized by: Indian Institute of Technology, Kanpur

Date: 8-12 December 2010

Papers presented

Title of the Presentation :

1. Structural and spectral properties of 4-bromo-1-naphthyl chalcones - A quantum chemical study
2. Studies on charge transport in π -stacked liquid crystalline molecules THDP and THDDP
3. Theoretical studies on absorption and emission properties of π -conjugated organic molecules
4. Theoretical Study of the second coordination sphere in 8-azaxanthinato salts of divalent metal aquacomplexes

Event: International Symposium of Molecules and Materials(A survey of recent concepts)

Organized by: Indian Institute of Science and Educational research (IISER), Kolkata

Date: 28-29 December 2009

Papers presented

Title of the Presentation : Theoretical studies on absorption and emission properties of π -conjugated organic molecules

Event: International Congress on Quantum Chemistry 2009

Organized by: Department of Chemistry, University of Helsinki, Helsinki, Finland

Date: 22-27 June 2009

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Alumini Reflections: