Bharathiar University

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

Dr L SENTHILKUMAR
Professor and Head
Department of Physics
Bharathiar University

Tamil Nadu
E-mail: lsenthilkumar@buc.edu.in
Phone: 9443702753
Office Number: 0422-2428443

Research Area

- 2D Materials
- Atmospheric Chemical Reaction
- Fuel Cell
- Carbon dioxide Reduction
- Ammonia Synthesis

Courses Teaching

- Quantum mechanics
- Mathematical Physics
- Solid State Physics
- Atomic Physics and Spectroscopy
- Research Methodology
- Molecular Quantum Mechanics

Research Experience: 19

Teaching Experience: 23

Research Credentials (as on February 2026 – Source: Google scholar)
H-index: 22 Citations: 2079 i10-index: 63

Publications
International Journals: 131

Career

At Bharathiar University

1. Designation : Professor
Period : March 2015 - Till Date

2. Designation : Associate Professor
Period : March 2012 - February 2015

Education

Ph. D.
Subject : Physics
Institution : Bharathiar University
Affiliated University : Bharathiar University
Year of Award : January 2007

M. Sc.
Subject : Physics
Institution : Bharathiar University
Affiliated University : Bharathiar University
Year of Award : May 1999

Projects
National Level
Ongoing - 1 completed - 4

Research Guidance
Completed
Ph.D. - 12 M.Phil. - 17 PG - 31

Institutional Responsibilities

Additional controller of Examination
Period :Aug 2018 - Dec 2024
Nature of Responsibility :

Deputy coordinator: UGC-SAP Program

Period :Feb 2015 to Till date

Nature of Responsibility :

Member, RUSA

Period :Jun 2016 - Jan 2018

Nature of Responsibility :

Member, Harassment complaint cell

Period :Jul 2018 - Jun 2019

Nature of Responsibility :

Visits

1. Visiting fellow, France (2015-10-30 - 2015-10-14)
2. Alternate Sponsored Fellowship, USA (2015-05-24 - 2015-05-18)
3. INSA Visiting Fellowship Award, Australia (2015-06-25 - 2014-06-28)

Publications

International Journals - 131

131. Structural Studies and Synthesis of a New 2-(1-Methyl-3-(o-tolyl)ureido)-N-(o-tolyl)acetamide: Binding Interaction With Bovine Gamma Globulin and DFT Investigation

Journal of Fluorescence (February 2026)

Arul Murugesan, Thangaraj Thiruppathiraja, Karuppasamy Nandhini, Krishnamoorthy Shanmugaraj, Senthilkumar Lakshmipathi, Malaichamy Ilanchelian

130. Tuning Emission Color: Substituent Controlled ESIPT and AIE enhancement in Hexafluoroisopropylidene Based Naphthyl Fluorophores for Live HeLa Cell Bioimaging

Dyes and Pigments (February 2026)

Moorthy Mathivanan, Thangaraj Thiruppathiraja, David Villaman, Jebiti Haribabu, Krishnamoorthy Shanmugaraj, Senthilkumar Lakshmipathi, Néstor Novoa

129. Cobalt manganese sulphide nanosheets: A Robust bifunctional catalyst for alkaline water electrolysis

Sustainable Energy & Fuels (February 2026)

Harshini Sharan, Angappan Kausalya, Senthilkumar Lakshmipathi, Pavithra Karthikesan, Jayachandran Madhavan, Alagiri Mani

128. Defect Engineering Coupled with N/O Co-Doping in Lignin-Derived Carbon for Enhanced ORR in Anion Exchange Membrane Fuel Cells

Carbon (November 2025)

Sabarinathan Ravichandran, Angappan Kausalya, Xinru Ji, Senthilkumar Lakshmipathi, Huaneng Su, Daifen Chen, Jie Yu

127. Electrochemical CO? Reduction to Methanol over Ni@Ti?CN MXene: A First-Principles DFT Study

Physical Chemistry Chemical Physics (November 2025)

Karthiga Manivannan; Senthilkumar Lakshmipathi

126. Fluorine and Amine Functionalized Co, Rh, and Ir-Doped Porphyrins for Oxygen Reduction and Hydrogen Evolution Catalysis: A DFT Study

Electrocatalysis (October 2025)

Angappan Kausalya, Senthilkumar Lakshmipathi

125. Edge carboxyl group functionalized RhN4-coronene as a catalyst for oxygen reduction and hydrogen evolution reactions: a DFT study

Theoretical Chemistry Accounts (October 2025)

Angappan Kausalya, Senthilkumar Lakshmipathi

Dr L SENTHILKUMAR , Professor and Head , Department of Physics

124. Molecular Self-recovery Features of Naphthyl Derivatives of Pyrimidine Bis Hydrazones: AIE, Mechanochromism and Al3+/Pyrophosphate (PPi) sensing

Dyes and Pigments (September 2025)
Ottoor Anitha, Janardhanan Aiswarya, Rajendran Kishore Kumar, Sandipan Ghorai, Thangaraj Thiruppathiraja, Ramalingam Natarajan, Senthilkumar Lakshmipathi, Balasubramanian Murugesapandian

123. Screening of Transition Metal (Sc to Zn) Decorated Mo3C2 MXenes as a Catalyst Under Ambient Conditions for N2 to NH3 Electrocatalysis Using First Principles Method

ChemPhysChem (September 2025)
Nandhini Panjulingam, Senthilkumar Lakshmipathi

122. Unveiling the Nickel?Manganese Sulfide Electrocatalyst for Enhanced Overall Alkaline Water Splitting

ACS Applied Energy Materials (August 2025)
Sharan Harshini, Kausalya Angappan, Senthilkumar Lakshmipathi, Madhavan Jayachandran, Karthikesan Pavithra, Mani Alagiri

121. Fe-decorated 2D AlN monolayers as sensor materials for octane and toluene molecules: a first-principles study

Physica Scripta (August 2025)
Surya Nagarathinam Senthilkumar, Senthilkumar Lakshmipathi

120. Electrocatalytic potential of bare and OH-functionalized Co-N-doped pyrene for ORR and HER: A DFT study

Computational and Theoretical Chemistry (June 2025)
Angappan Kausalya, Thangaraj Thiruppathiraja, Senthilkumar Lakshmipathi

119. Construction of Cu-MOF@Bi2MoO6 Z-scheme heterostructure mediated by Bi nanoparticles and oxygen vacancies for ciprofloxacin degradation and mechanism investigation

Environmental Science: Nano (June 2025)
Senthilkumar Lakshmipathi and Tae Hwan Oh Ranjith Kumar Dharman, Angappan Kausalya, Stella Vargheese

118. Blue (Buckled) Versus Black (Puckered) Phosphorene Monolayers for Sensing Biomarkers Associated with Respiratory Diseases – A DFT Study

Advanced Theory and Simulations (May 2025)
Senthilkumar Surya, Nagarathinam, Lakshmipathi Senthilkumar

117. Poly((biphenyl)m-(aryl methylpiperidine)n-(dibenzothiophene)p)-Based Proton Exchange Membrane for High-Temperature Fuel Cell Application

ACS Applied Polymer Materials (May 2025)
Divya Kumar, Murali Ravi, qing qing liu, Huiyuan Liu, Thangaraj Thiruppathiraja, Weiqi Zhang, Qian Xu, Senthilkumar Lakshmipathi, Huaneng Su

116. A novel chemical probes with innovative ZnO nanoparticle designs for precise detection of Cd2+, Hg2+ and H2PO4-Ions: DFT insights and molecular logic gate applications

Journal of Molecular Structure (April 2025)
G Tamilselvan, T Thiruppathiraja, V Srinivasadesikan, A Ravikumar, A Arunjegan, Xuesong Li, S Lakshmipathi, Paulraj Mosae Selvakumar, Zhen Zhang, Hongjun Zhao

115. pH impact on bismuth vanadate nanomaterial: Photocatalyst and supercapacitor application

Ceramics International (April 2025)
Yamuna Radhakrishnan, R Karunathan, Nandhini Panjulingam, Senthilkumar Lakshmipathi, Babu Balraj, Chandrasekar Sivakumar

114. Aminothiophenol and 7-diethylamino-4-hydroxycoumarin derived probe for reversible turn off–on–off detection of Cu2+ ions and cysteine

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy (February 2025)
Kuppusamy Suganthirani, Thangaraj Thiruppathiraja, Senthilkumar Lakshmipathi, Jan Grzegorz Malecki, Balasubramanian Murugesapandian

Dr L SENTHILKUMAR , Professor and Head , Department of Physics

113. AIE active hydroxycoumarin-anthranilic acid coupled enamine: Sequential detection of Cu2+/S2? ions and live cell imaging application

Microchemical Journal (December 2024)
Kuppusamy Suganthirani, Rajendran Kishore Kumar, Thangaraj Thiruppathiraja, Panneerselvan Prabha, Senthilkumar Lakshmipathi, Subramaniam Selvakumar, Jan Grzegorz Malecki, Balasubramanian Murugesapandian

112. 2D MoS2 for Detection of COVID-19 Biomarkers–A First-Principles Study

Physica Scripta (December 2024)
Surya Nagarathinam Senthilkumar, Nandhini Panjulingam, Senthilkumar Lakshmipathi

111. 2D Co-anti-MXenes (CoB/CoP) as promising anode materials for magnesium-ion batteries in diglyme and triglyme electrolytes: a first-principles study

Physical Chemistry Chemical Physics (December 2024)
Nandhini Panjulingam, Senthilkumar Lakshmipathi

110. Reduction of N2 to NH3 using FeP (101)/TiO2 catalysts: A First-principles study

International Journal of Hydrogen Energy (November 2024)
Nandhini Panjulingam, Senthilkumar Lakshmipathi

109. Versatile aggregation induced emissive molecular probes incorporating different donor/acceptor groups for tunable multiple color fluorescence

Dyes and Pigments (September 2024)
Moorthy Mathivanan, David Villaman, Krishnamoorthy Shanmugaraj , Malaichamy Ilanchelian , Thangaraj Thiruppathiraja , Senthilkumar Lakshmipathi, Néstor Novoa

108. Pyridine appended pyrimidine bis hydrazone: Zn2+/ATP detection, bioimaging and functional properties of its dinuclear Zn (II) complex

Talanta (July 2024)
Ottoor Anitha, Sandipan Ghorai, Thangaraj Thiruppathiraja, Humayun Amir, Abinayaselvi Murugan, Ramalingam Natarajan, Senthilkumar Lakshmipathi, Chinnuswamy Viswanathan, Mathivanan Jothi, Balasubramanian Murugesapandian

107. Density functional theory analysis of iodine coadsorbed OH-copper phthalocyanine for dopamine sensing

Molecular Physics (July 2024)
Sangeetha Thekkayil L. Senthilkumar

106. 2D g-GaN as interphase anode layer in Mg battery for capturing passivation species (MgO, Mg(OH)2, MgCO3) — A first-principles study

Ionics (June 2024)
N Panjulingam, S Lakshmipathi

105. Highly sensitive prismatic h-MoO3 sheets for temperature-dependent chemiresistive ammonia sensor

Journal of Materials Science: Materials in Electronics (April 2024)
K Muthumalai, Nandhini Panjulingam, Mathankumar Manoharan, Kamaraj Govindharaj, Poovarasan Saravanan, Senthilkumar Lakshmipathi, Yuvaraj Haldorai, Ramasamy Thangavelu Rajendra Kumar

104. OH-Functionalized N-Doped Graphene Quantum Dots as an Efficient Metal-Free Catalysts for Oxygen Reduction Reaction in PEMFCs

Electrocatalysis (April 2024)
Thangaraj Thiruppathiraja, Senthilkumar Lakshmipathi

103. Dopamine adsorption on OH-functionalized metal phthalocyanines [MPc](M= Mg, Co) in gas and solvent (water, ethanol) medium: A DFT study

Computational and Theoretical Chemistry (March 2024)
Thekkayil Sangeetha, Senthilkumar Lakshmipathi

102. Exploring the potential of alkali metal-decorated TPH-Graphene nanoribbons for high-efficiency hydrogen storage: A first-principles study

International Journal of Hydrogen Energy (February 2024)
Umadevi Palanivel, Vijayakumar Elayappan, Senthilkumar Lakshmipathi

Dr L SENTHILKUMAR , Professor and Head , Department of Physics

101. Vanadium doped B5N3 and B7N5 monolayer as single atom catalyst for nitrogen reduction reaction – a first-principles study

Molecular Physics (February 2024)
Nandhini Panjulingam, Senthilkumar Lakshmipathi

100. Diethylaminophenol appended pyrimidine bis hydrazone for the sequential detection of Al3+ and PPi ions

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy (December 2023)
Ottoor Anitha, Thangaraj Thiruppathiraja, Senthilkumar Lakshmipathi, Balasubramanian Murugesapandian

99. N-piperidinyl substituted trioxotriangulene as an efficient catalyst for oxygen reduction reaction in fuel cell application—a DFT study

Ionics (December 2023)
Thangaraj Thiruppathiraja, Senthilkumar Lakshmipathi

98. Interfacial oxygen vacancy modulated ZIF-8-derived ZnO/CuS for the photocatalytic degradation of antibiotic and organic pollutants: DFT calculation and degradation pathways

Chemical Engineering Journal (November 2023)
Athibala Mariappan, Pandian Mannu, Thangaraj Thiruppathiraja, Ta Thi Thuy Nga, Senthilkumar Lakshmipathi, Chung-Li Dong, Ranjith Kumar Dharman, Tae Hwan Oh

97. Multiphase MoS2 monolayer: A promising anode material for Mg-Ion batteries

Ionics (September 2023)
Nandhini Panjulingam, Senthilkumar Lakshmipathi

96. Microwave Hantzsch Synthesis of Quinolinyl-Dihydropyridines Supported by Cs-BNT Catalyst and DFT Investigations

Polycyclic Aromatic Compounds (September 2023)
Sureshkumar Mahalingam, Ephraim Muriithi Kiarii, Thangaraj Thiruppathiraja, Arul Murugesan, Senthilkumar Lakshmipathi, Talent Raymond Makhanya, Robert M Gengan

95. An AIE active acidochromic pyrimidine-functionalized two-in-one fluorescent probe for selective relay detection of Al 3+/Zn 2+ and PPi with various detection applications

New Journal of Chemistry (September 2023)
Ottoor Anitha, Janardhanan Aiswarya, Thangaraj Thiruppathiraja, Senthilkumar Lakshmipathi, Jan Grzegorz Ma?ecki, Balasubramanian Murugesapandian

94. Reaction mechanism of methyl trifluoroacetate (CH3TFA) with lithium polysulfides (Li2S6) in gas and solvent phase

Theoretical Chemistry Accounts (September 2023)
Meera Cheviri, Senthilkumar Lakshmipathi

93. Shear-induced symmetry-breaking dynamical states

The European Physical Journal Plus (August 2023)
K Premalatha, VK Chandrasekar, L Senthilkumar, M Lakshmanan

92. Visualization of latent fingerprints using an AIE-active unsymmetrical azine: 2-Naphthol-pyrrole acrylate conjugate and its fluorescent sensing of Cu2+ and S2? ions, smartphone and logic gate applications

Journal of Photochemistry and Photobiology A: Chemistry (August 2023)
Balamurugan Tharmalingam, Ottoor Anitha, Janardhanan Aiswarya, Thangaraj Thiruppathiraja, Senthilkumar Lakshmipathi, Balasubramanian Murugesapandian

91. A first-principles study on chemical adsorption of lithium polysulfide molecules: investigating the influence of carbon, boron, and nitrogen vacancies in boron carbon nitride 2D sheets

Applied Physics A (July 2023)
Meera Cheviri, Senthilkumar Lakshmipathi

90. A unique methanol responsiveness, AIE, acidochromism and mechanofluorochromic features of flexible ethylenediamine bridged rhodamine B-diethylamino hydroxycoumarin conjugate

Journal of Molecular Liquids (July 2023)
Mathivanan Moorthy, Tharmalingam Balamurugan, Anitha Ottoor, Thiruppathiraja Thangaraj, Lakshmipathi Senthilkumar, Ma?ecki Jan Grzegorz, Balasubramanian Murugesapandian

Dr L SENTHILKUMAR , Professor and Head , Department of Physics

89. DFT Study on a Fluorine-Functionalized Nitrogen-and Boron-doped Triangulene as an Electrocatalyst for the Oxygen Reduction Reaction

Sustainable Energy & Fuels (May 2023)
Thangaraj Thiruppathiraja, Pugal Neelam Parameswaran Senthan, Senthilkumar Lakshmipathi

88. Reaction mechanism and kinetics of H and Cl atom abstraction in Dichloromethane with OH radical

Computational and Theoretical Chemistry (May 2023)
Angappan Mano Priya, Basheer Aazaad, Vasanth Perumal Mythili, Senthilkumar Lakshmipathi

87. Multi-stimuli responsiveness of pyrimidine bishydrazone: AIE, tuneable luminescence, white light emission, mechanochromism, acidochromism and its anticounterfeiting applications

Dyes and Pigments (April 2023)
Ottoor Anitha, Moorthy Mathivanan, Balamurugan Tharmalingam, Thangaraj Thiruppathiraja, Sandipan Ghorai, Ramalingam Natarajan, Viruthachalam Thiagarajan, Senthilkumar

86. Catalytic activity of OH functionalized N-doped graphene in oxygen reduction reaction for fuel cell applications: a DFT study

Applied Physics A (February 2023)
Thangaraj Thiruppathiraja, Senthilkumar Lakshmipathi

85. Intramolecular Interactions (OH••• O, CH••• N, NH••• ?) in Isomers of Neutral, Cation, and Anion Dopamine Molecules-A DFT Study on the Influence of Solvents (Water and Ethanol)

Journal of Molecular Modeling (February 2023)
Thekkayil Sangeetha, Senthilkumar Lakshmipathi

84. Detection of nonpolar n-dodecane at room temperature using multiphase MoS2 chemiresistive sensor: Investigation of charge transfer on nonpolar VOC molecule

Sensors and Actuators B: Chemical (February 2023)
K Muthumalai, Nandhini Panjulingam, Mathankumar Manoharan, Yuvaraj Haldorai, Senthilkumar Lakshmipathi, Ramasamy Thangavelu Rajendra Kumar

83. Green synthesis of benzimidazole derivatives by using zinc boron nitride catalyst and their application from DFT (B3LYP) study

Heliyon (November 2022)
Sureshkumar Mahalingam, Arul Murugesan, Thangaraj Thiruppathiraja, Senthilkumar Lakshmipathi, Talent Raymond Makhanya, Robert M Gengan

82. Redox induced electron transfer in lithium polysulfide–A DFT study

Journal of Sulfur Chemistry (September 2022)
Meera Cheviri, Senthilkumar Lakshmipathi.

81. Experimental and Theoretical Analysis of Synthesized Poly-(pthalazinone ether sulfone ketone) Copolymer Modified Separators for Li-S Batteries

ChemElectroChem (August 2022)
Mathivanan Tamilarasan, Subrata Dolui, Nandhini Panjulingam, Rajkumar Kanakaraj, Lakshmipathi Senthilkumar, Banerjee ,Sanjib, Kalai Selvan Ramakrishnan

80. Investigation of the Gas?Phase Reaction of Nopinone with OH Radicals: Experimental and Theoretical Study

Atmosphere (August 2022)
Gisèle El Dib, Angappan Mano Priya, Senthilkumar Lakshmipathi

79. Enhancement of electrochemical performances of Li-S batteries using PPESK and Nelumbo nucifera derived porous carbon modified separator

Materials Letters (May 2022)
Tamilarasan Mathivanan, Nandhini Panjulingam, Subrata Dolui, Senthilkumar Lakshmipathi, Sanjib Banerjee, Ramakrishnan Kalai Selvan

Dr L SENTHILKUMAR , Professor and Head , Department of Physics

78. Experimental and Theoretical Studies of Trans-2-Pentenal Atmospheric Ozonolysis

Atmosphere (February 2022)
Kalalian Carmen, Grira Asma, Niklas Illmann Jan, Patroescu-Klotz Iulia, El Dib Gisèle, Coddeville Patrice, Canosa André, Wiesen Peter, Aazaad Basheer, Senthilkumar Lakshmipathi, Estelle Roth, Tomas Alexandre, Chakir Abdelkhaleq

77. Pyrrolic, pyridinic, and graphitic sumanene as metal-free catalyst for oxygen reduction reaction – A density functional theory study

Fuel Cells (November 2021)
Thiruppathiraja Thangaraj, Arokiyanathan Agnes Lincy, Lakshmipathi Senthilkumar

76. Complexes of criegee intermediate CH2OO with CO, CO2, H2O, SO2, NO2, CH3OH, HCOOH and CH3CH3CO molecules – A DFT study on bonding, energetics and spectra

Computational and Theoretical Chemistry (September 2021)
Shyama Muraledharan, Cheviri Meera, Mano Priya Angappan, Lakshmipathi Senthilkumar

75. Nitrogen-Doped Buckybowls as Potential Scaffold Material for Lithium-Sulfur Battery: A DFT Study

Electrocatalysis (August 2021)
Meera Cheviri, Senthilkumar Lakshmipathi

74. DFT Study of Chemical Reactivity Parameters of Lithium Polysulfide Molecules Li2Sn (1?n?8) in Gas and Solvent phase

Computational and Theoretical Chemistry (August 2021)
M Cheviri, L. Senthilkumar

73. Adsorption properties of amino acid-based ionic liquids (AAILs) on edge fluorinated graphene surface – a DFT study

Molecular Simulation (June 2021)
Shyama Muraledharan, Lakshmipathi Senthilkumar

72. Cation-Anion Interactions, Stability, and IR Spectra of Dicationic Amino Acid-Based Ionic Liquids...

Journal of Molecular Modeling (May 2021)
S Muraledharan, L. Senthilkumar

71. Theoretical perspective on the interaction of CO 2 and H 2 O molecules with functionalized...

Theoretical Chemistry Accounts (March 2021)
AL Arokiyanathan, L. Senthilkumar

70. Synthesis of metal-free nitrogen-enriched porous carbon and its electrochemical sensing...

Materials Chemistry and Physics (February 2021)
P RupaKasturi, TK Aparna, AL Arokiyanathan, L. Senthilkumar, Ramanathan Sivasubramanian, Yun Sung Lee, Ramakrishnan KalaiSelvan

69. Glutathione functionalized Copper Nanoclusters as a Fluorescence Platform for Specific Biosensing...

Microchemical Journal (November 2020)
R Ramar, A Basheer, L. Senthilkumar, I Malaichamy

68. Water confined (H2O) n= 1–10 amino acid-based ionic liquids–a DFT study on the bonding, energetics and IR spectra

Journal of Molecular Liquids (April 2020)
M Shyama, L. Senthilkumar

67. Chemical Properties of Lithium Cluster (Lix x= 2-8) On Stone-Wales Defect Graphene Sheet-A DFT Study

The Journal of Physical Chemistry C (March 2020)
AL Arokiyanathan, N Panjulingam, L. Senthilkumar

66. H, OH and COOH functionalized magnesium phthalocyanine as a catalyst for oxygen reduction ...

International Journal of Hydrogen Energy (March 2020)
T Thangaraj, A Agnes Lincy, A Basheer, S Ramesh, L. Senthilkumar

65. Cobalt phthalocyanine is a suitable scaffold for lithium polysulfide (Li2Sn n= 2–8)

Chemical Physics Letters (January 2020)
M Cheviri, L. Senthilkumar

Dr L SENTHILKUMAR , Professor and Head , Department of Physics

64. Effect of metal substitution (Mg, Sc) and functionalization (H, F, NH2, CH3, OH, CHO, and COOH) on the absorption properties of phthalocyanines – A TDDFT study

Polyhedron (January 2020)
Agnes LincyArokiyanathan, L. Senthilkumar

63. ZnO and TiO2 clusters as catalyst in the addition and abstraction reaction of acrylic acid with the OH radical

International Journal of Chemical Kinetics (October 2019)
Basheer Aazaad, L. Senthilkumar

62. Adsorption and sensing properties of non-planar ? surfaces towards high energy molecules...

Journal of Physics and Chemistry of Solids (September 2019)
L. Senthilkumar, Agnes Lincy Arokiyanathan Vidhyashree Ramasamy

61. C–H···O interaction between cation and anion in amino acid-based ionic liquids—A DFT study in gas and solvent phase

Structural Chemistry (February 2019)
Shyama Muraledharan, L. Senthilkumar

60. Impact of Functional Groups Substitution on the Molecular Properties of Magnesium and Scandium Phthalocyanines

Inorganica Chimica Acta (November 2018)
Agnes Lincy. A, L. Senthilkumar

59. OH initiated oxidation mechanism of monoterpene (linalool) – A first comprehensive theoretical study

Atmospheric Environment (September 2018)
Basheer Aazaad , L. Senthilkumar

58. The first-principles study of CoSb2O4 and its electrochemical properties for supercapacitors

Electrochimca Acta (September 2018)
Amirthalingam Shanmugavani, Murugan Lalitha, Rajeesh Kumar Narayanan Kutty, Leonid Vasylechko, Yun Sung Lee, L. Senthilkumar, Ramakrishnan Kalai Selvan

57. An Experimental and Theoretical Study on the Kinetics of the Reaction between 4-Hydroxy-3-Hexanone H3CH2C(O)CH(OH)CH2CH3...

International Journal of Chemical Kinetics (June 2018)
Gisèle El Dib, Basheer Aazaad , L. Senthilkumar, Hélène Laversin, Estelle Roth, Abdelkhaleq Chakir

56. Theoretical Study on the Interaction of CO2 and H2O molecules with Metal doped-Fluorinated Phthalocyanines

New Journal of Chemistry (June 2018)
Agnes Lincy. A, L. Senthilkumar

55. Molecular Properties of Metal Difluorides and their Interaction with CO2, H2O molecules - A DFT Investigation

Journal of Molecular Modeling (November 2017)
Agnes Lincy. A , L. Senthilkumar

54. Gas adsorption efficacy of graphene sheets functionalised with carboxyl, hydroxyl and epoxy groups in conjunction with Stone–Thrower–Wales (STW) and inverse Stone–Thrower–Wales (ISTW) defects

Phys. Chem. Chem. Phys. (October 2017)
Murugan Lalitha, L. Senthilkumar

53. Experimental and theoretical investigations of the kinetics and mechanism of the Cl+ 4-hydroxy-4-methyl-2-pentanone reaction

Atmospheric environment (October 2017)
L Aslan, A Mano Priya, C Sleiman, MN Zeineddine, Patrice Coddeville, Christa Fittschen, B Ballesteros, André Canosa, L Senthilkumar, G El Dib, A Tomas

Dr L SENTHILKUMAR , Professor and Head , Department of Physics

52. Improved Lithium adsorption in Boron and Nitrogen-substituted Graphene derivatives

Journal of Material Science (September 2017)
M. Lalitha, S.Selva Mahadevan, L. Senthilkumar

51. Reaction of Pentanol isomers with OH radical – A theoretical perspective

Molecular Physics (August 2017)
B. Aazaad, L. Senthilkumar

50. Facile Hydrothermal Synthesis and First Principle Computational Studies of NiSb2O4 and Its Electrochemical Properties with Ni3(Fe(CN)6)2(H2O) for Hybrid Supercapacitors

Chemistry Select (August 2017)
Amirthalingam Shanmugavani, Murugan Lalitha, Subramanian Yuvaraj, Leonid Vasylechko, Danielle Meyrick, Lakshmipathi Senthilkumar, Ramakrishnan Kalai Selvan

49. Interface energetics of [Emim]+[X]? and [Bmim]+[X]? (X = BF4, Cl, PF6, TfO, Tf2N) based ionic liquids on graphene, defective graphene, and graphyne surfaces

Journal of Molecular Liquids (June 2017)
Lalitha Murugan, Lakshmipathi Senthilkumar

48. Adsorption behaviour of reduced graphene oxide towards cationic and anionic dyes: Co-action of electrostatic and ? – ? interactions

Materials Chemistry and Physics (June 2017)
Ramasamy Thangavelu Rajendra Kumar Cherukutty Ramakrishnan Minitha, Murugan Lalitha, Yekkoni Lakshmanan Jeyachandran, Lakshmipathi Senthilkumar

47. DFT study on abstraction reaction mechanism of oh radical with 2-methoxyphenol

Journal of Physical Organic Chemistry (May 2017)
A.Manopriya, L. Senthilkumar

46. Atmospheric fate of diketones and OH radical–kinetics, reaction force, ETS-NOCV analysis

Molecular Physics (April 2017)
Mano Priya Angappan, Lakshmipathi Senthilkumar

45. Edge functionalised & Li-intercalated 555-777 defective bilayer graphene for the adsorption of CO2 and H2O

Applied Surface Science (April 2017)
M. Lalitha, L. Senthilkumar, Suresh K. Bhatia

44. Elucidation of Binding Mechanism of Photodynamic Therapeutic Agent Toluidine Blue O with Chicken Egg White Lysozyme by Spectroscopic and Molecular Dynamics Studies

Photochemistry and Photobiology (March 2017)
Shanmugaraj Krishnamoorthy, Umadevi Palanivel, Senthilkumar Lakshmipathi, Ilanchelian Malaichamy

43. Reaction of NO3 radical with benzyl alcohol - A DFT study

Computational and Theoretical Chemistry (February 2017)
Basheer Aazaad, L. Senthilkumar

42. Interaction between Arginine conformers and Hofmeister Halide anions

Computational and Theoretical Chemistry (November 2016)
P Umadevi, L Senthilkumar

41. Influence of dopants Cu, Ga, In, Hg on the electronic structure of CdnSn (n = 6, 15) clusters – a DFT study

RSC Advances (September 2016)
paramasivam ganesan, Senthilkumar lakshmipathi

40. Addition and abstraction reaction mechnanism of 2,4,5 Trimethylphenol with OH radical - A First Principle study

Computational and Theoretical Chemistry (September 2016)
Basheer Azaad, A.Mano Priya, L. Senthilkumar

Dr L SENTHILKUMAR , Professor and Head , Department of Physics

39. Impact of heterogeneous passivation of trimethylphosphine oxide and di-methylphosphine oxide surface ligands on the electronic structure of CdnSen (n=6, 15) quantum dots: A DFT study

Physica E: Low-dimensional Systems and Nanostructures (September 2016)
Parasivam Ganesan, Senthilkumar Lakshmipathi

38. First Experimental and Theoretical Kinetic Study of the Reaction of 4-Hydroxy-4-methyl 2-pentanone as a Function of Temperature

International Journal of chemical Kinetics (July 2016)
Mano Priya Angappan, Lakshmipathi Senthilkumar, Chakir Abdelkhaleq, El Dib Gisèle

37. Calcium Decorated and Doped Phosphorene for Gas Adsorption

Applied Surface Science (July 2016)
M lalitha, Y Natara, j S Lakshmipathi

36. Hydrogen bonds in Zif268 proteins – a theoretical perspective

Journal of Biomolecular Structure and Dynamics (May 2016)
P Umadevi, L. Senthilkumar

35. Metal interacted Histidine Dimer- An ETS-NOCV and XANES Study

RSC Advances (April 2016)
P Umadevi, L. Senthilkumar

34. Theoretical studies on interaction of anticancer drugs (dacarbazine, procarbazine and triethylenemelamine) with normal (AT and GC) and mismatch (GG, CC, AA and TT) base pairs

Molecular Simulation (December 2015)
R. Shankar, R. Radhika, D. Thangamani, L. Senthil kumar, & P. Kolandaivel

33. The influence of interfaces and intra-band transitions on the band gap of CdS/HgS and GaN/X (X= InN, In0.33Ga0.67N) core/shell/shell quantum dot quantum well–A theoretical study

Physica E: Low-dimensional Systems and Nanostructures (November 2015)
P Ganesan, L Senthilkumar

32. Multi walled Carbon Nanotube Oxygen Sensor: Enhanced Oxygen Sensitivity at Room Temperature and Mechanism of Sensing

ACS Applied Materials & Interfaces (October 2015)
Raja Vel, Lalitha Murugan, Radhakrishnan Jogee Kullan, Senthilkumar Lakshmipathi, Rajendra Kumar Ramasamy Thangavelu

31. DFT study on the tautomerism of organic linker 1H- Imidazole-4,5-Tetrazole (HIT)

Computational and Theoretical Chemistry (September 2015)
V. Umadevi, A. Mano Priya, L. Senthilkumar

30. Defect-mediated reduction in barrier for helium tunneling through functionalized graphene nanopores

The Journal of Physical Chemistry C (August 2015)
M. Lalitha, L. Senthilkumar, Suresh K Bhatia

29. Encapsulation of fluroethanols in pristine and stone-wales defect boronnitride nanotube- A DFT Study

Applied Surface Science (August 2015)
P Umadevi, T Aiswarya, L. Senthilkumar

28. Study on the I–V characteristics of quantum well/dot embedded GaAs/AlGaAs structures - A transfer matrix method

AIP Conference Proceedings (August 2015)
P. Ganesan; K. Vanitha; L. Senthilkumar

27. Effect of alkyl chain on the NLO property of nonylphenol isomers: a DFT study

Monatshefte für Chemie (June 2015)
V Umadevi, P Umadevi, N Santhanamoorthi, L Senthilkumar

26. Reaction of OH radical and ozone with methyl salicylate – a DFT study

Journal of Physical Organic Chemistry (April 2015)
A. Mano Priya and L. Senthilkumar

Dr L SENTHILKUMAR , Professor and Head , Department of Physics

25. An experimental and theoretical study of the kinetics of the reaction between 3-hydroxy-3-methyl-2-butanone and OH radicals

Rsc Advances (March 2015)
Angappan Mano Priya, Gisèle El Dib, Lakshmipathi Senthilkumar, Chantal Sleiman, Alexandre Tomas, André Canosa, Abdelkhaleq Chakir

24. DFT study on X?.(H2O)n=1-10 (X=OH, NO2, NO3, CO3) anionic water Cluster

Journal of Molecular Graphics and Modelling (November 2014)
M.Lalitha, L. Senthilkumar

23. Structure and NLO properties of halogen (F, Cl) substituted formic acid dimers.

Spectrochimica Acta Part A (November 2014)
P. Umadevi, L. Senthilkumar, M.Gayathri, P. Kolandaivel

22. Influence of metal ions (Zn2+, Cu2+, Ca2+, Mg2+ and Na+) on the water coordinated neutral and zwitterionic L-Histidine dimer

RSC Advances (September 2014)
P Umadevi, L Senthilkumar

21. Influence of In-plane Stone-Thrower-Wales Defects and Edge Functionalisation on the Adsorption of CO2 and H2O on Graphene

RSC Advances (August 2014)
Lalitha Murugan, Senthilkumar Lakshmipathi, Suresh K. Bhatia

20. Photoactive amorphous molecular materials based on bisquinoline diamines and their synthesis by Friedländer condensation reaction

Journal of Photochemistry and Photobiology A: Chemistry (June 2014)
Pradip K. Bhowmik a, Alexi K. Nedeltchev a, Haesook Han a, Tae Soo Jo a, Jung Jae Koh a, Lakshmipathi Senthilkumar b, Palanivel Umadevi b

19. Degradation of methyl salicylate through Cl initiated atmospheric oxidation – theoretical study

RSC Advances (May 2014)
A.Mano Priya, L. Senthilkumar

18. Understanding Molecular properties of halogenated cyclohexane- A DFT study

Computational and Theoretical Chemistry (April 2014)
V. Umadevi, N. Santhanamoorthi , L. Senthilkumar

17. Hydrogen-bond interactions in hydrated 6-selenoguanine tautomers: a theoretical study

Structural Chemistry (April 2014)
M. Karthika, L. Senthilkumar & R. Kanakaraju

16. Hydrogen-bonded complexes of serotonin with methanol and ethanol: A DFT study

Structural Chemistry (February 2014)
A. Mano Priya, L. Senthilkumar & P. Kolandaivel

15. Density functional theory investigation of cocaine water complexes

Journal of molecular modeling (May 2013)
Lakshmipathi Senthilkumar, Palanivel Umadevi, Kumaranathapuram Natarajan Sweety Nithya, Ponmalai Kolandaivel

14. Theoretical investigations on the hydrogen bonding of nitrile isomers with H2O, HF, NH3 and H2S

Molecular Simulation (April 2013)
V Umadevi, L Senthilkumar, P Kolandaivel

13. Spectroscopic investigations and hydrogen bond interactions of 8-aza analogues of xanthine, theophylline and caffeine: a theoretical study

Journal of molecular modeling (January 2013)
Mylsamy Karthika, Ramasamy Kanakaraju, Lakshmipathi Senthilkumar

12. The study of performance of DFT functional for van der Waals interactions

Computational and Theoretical Chemistry (January 2013)
P Kolandaivel, D Uma Maheswari, L Senthilkumar

11. Coordination and binding properties of zwitterionic glutathione with transition metal cations

Inorganica Chimca acta (May 2012)
R Shankar, P. Kolandaivel, L Senthil Kumar

10. Hydrogen?bonded complexes of nicotine with simple alcohols

International Journal of Quantum Chemistry (January 2012)
Lakshmipathi Senthilkumar, Tapan K Ghanty, Ponmalai Kolandaivel, Swapan K Ghosh

9. Theoretical investigations on hydrated 6, 8-dithioguanine tautomers

Structural Chemistry (January 2012)
M Karthika, L Senthilkumar, R Kanakaraju

8. Theoretical studies on hydrogen bonding in caffeine–theophylline complexes

computational and theoretical chemistry (January 2012)
M Karthika, L Senthilkumar, R Kanakaraju

7. Interaction studies of cysteine with Li+, Na+, K+, Be2+, Mg2+, and Ca2+ metal cation complexes

Journal of Physical Organic Chemistry (February 2011)
R Shankar, P Kolandaivel, L Senthilkumar

6. Importance of hydrogen bonding for second harmonic generation effect: X-ray diffraction and DFT study on S-benzyl isothiouronium chloride

Journal of Physics and Chemistry of Solids (February 2009)
P Hemalatha, V Veeravazhuthi, D Velmurugan, L Senthilkumar, J Mallika, D Mangalaraj

5. Hydrogen bonding in substituted formic acid dimers

The Journal of Physical Chemistry A (November 2006)
L Senthilkumar, Tapan K Ghanty, Swapan K Ghosh, P Kolandaivel

4. Molecular interaction study of formohydroxamic acid (FHA) with water

Journal of molecular structure (June 2006)
L Senthilkumar, P Kolandaivel

3. Electron density and energy decomposition analysis in hydrogen-bonded complexes of azabenzenes with water, acetamide, and thioacetamide

The Journal of Physical Chemistry A (August 2005)
L Senthilkumar, Tapan K Ghanty, Swapan K Ghosh

2. Study of effective hardness and condensed Fukui functions using AIM, ab initio, and DFT methods

Molecular Physics (February 2005)
L Senthilkumar, P Kolandaivel*

1. Post Hartree–Fock and density functional theory studies on tautomerism of 6-thioxanthine in gas phase and in solution

Journal of Molecular Structure: THEOCHEM (October 2003)
L Senthilkumar, P Kolandaivel

Projects

Completed - 4

1. Theoretical Investigations on the pure and metallated Protein-DNA interactions DST – SERB Rs. 8.13 Lakhs (January 2012 - January 2016)

2. Investigations on integrated system of Fluorinated-Graphene+ Amino Acid-based ionic Liquids for CO2 capture DST – SERB Rs. 35.56 Lakhs (February 2017 - February 2020)

3. Metal Organic functionalised 2D MoS2, WS4 based electronic nose towards selective detection of disease related Volatile Organic Compounds DST – SERB Rs. 39.85 Lakhs (September 2018 - September 2021)

4. Investigation on the Reduction of Polysulfide Shuttling Effect Using Electrospun Polymer Composite Membrane Separators for High-Performance Li- S batteries DST – SERB Rs. 37.42 Lakhs (March 2019 - March 2022)

Ongoing - 1

1. "2-Dimensional Materials for Covid-19 Breath Analyzer- A DFT Study" DST – SERB Rs. 29.53 Lakhs (March 2022 - March 2025)