




Bharathiar University

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<p>Research Area</p> <ul style="list-style-type: none"> • 2D Materials for Energy and Environmental Applications • Degradation of Hazardous Atmospheric Reactions • Biomolecular interactions 	<p>Courses Teaching</p> <ul style="list-style-type: none"> • Classical Mechanics • Quantum Mechanics • Energy Resources • Numerical Methods • Statistical and Thermodynamics
<p>Research Experience: 18</p>	<p>Teaching Experience: 15</p>
<p>Research Credentials (as on September 2025 – Source: Google scholar) H-index: 1980 Citations: 25 i10-index: 57</p>	
<p>Publications International Journals: 116</p>	
<p>Publications</p> <p>International Journals - 116</p> <p>116. Activating the quantum capacitance of C24 Nanocages for supercapacitors through B/N substitution and 3d transition metal doping (Scsingle bondZn) - a DFT perspective</p> <p>Diamond and Related Materials, Volume 163, 113398 (February 2026) Divyakaaviri Subramani a , Akilesh Muralidharan a , Shamini Pazhani Beena a , Shankar Ramasamy</p> <p>115. Morphology-phase coupled engineering of NiCuCo layered double hydroxide towards efficient alkaline overall water splitting</p> <p>Fuel, Volume 417, Pages 138613 (February 2026) Jayachandran Madhavan, Deepak Arumugam, Sugasri Chinnasamy, Pavithra Karthikesan, Harshini Sharan, Shankar Ramasamy, Puviyarasi Balakrishnan, Alagiri Mani</p> <p>114. Enhanced electrochemical performance of ammonium phosphomolybdate for symmetric and asymmetric supercapacitors in an H₂SO₄/KI redox additive electrolyte</p> <p>Nanoscale (January 2026) S Mohammed Eliyas, R Yuvakkumar, G Ravi, A Deepak, R Shankar, Dhayalan Velauthapillai</p> <p>113. Bromoamination of α,β-unsaturated keto alkenes by palladium (ii) metalloalicycles: experimental and theoretical approaches</p> <p>New Journal of Chemistry, Volume 50, Issue 3, Pages 1602-1612 (January 2026) S Nandhini, S Dharani, B Mugesh, G Prabusankar, S Mohanapriya, R Shankar, R Prabhakaran</p> <p>112. Unveiling the influence of 3d transition metal (Sc–Zn) doping on quantum capacitance and surface charge storage in bare nano cages (Al12N12, Al12P12, B12N12, and B12P12) – a first principles simulation study</p> <p>Physical Chemistry Chemical Physics (January 2026) Divyakaaviri Subramani, Deepak Arumugam ORCID logo, Akilesh Muralidharan, Shamini Pazhani Beena and Shankar Ramasamy</p>	



111. Design and synthesis of 8-nitroquinoline azine D-?-A module chemosensors: Fluorogenic onsite detection of sarin gas mimic-DCP

Talanta Open, Volume 12, Pages 100508 (December 2025)

Sentamil Selvi Ramasamy, Kaviyarasu Adhigaman, Vandana Nandakumar, Akilesh Muralidharan, Shankar Ramasamy, Suresh Thangaraj

110. A Dual Signalling On-Off Quinoline Imidazole Conjugate: a Fluorescent Chemosensor for Fe²⁺ and Hg²⁺ Ions and Bioimaging Studies

Journal of Fluorescence, Pages 1-12 (November 2025)

Arumugam Sreedevi, Ramasamy Shankar, Gopalan Subashini

109. Designing Biobased Sulfur-Modified Benzoxazines for Enhanced Performance in Antimicrobials, Anticorrosion, and Dielectrics

ACS Applied Polymer Materials, volume 7, issue 21, 15075–15089 (October 2025)

Mohamed Mydeen KHarinei SrinivasanSubasri AppasamyBalaji Krishnasamy*Shankar Ramasamy

108. Experimental investigations and DFT insights of atmospheric DBD plasma-induced surface modifications in curcumin-loaded PVA and chitosan films for bio-medical applications

International Journal of Biological Macromolecules Volume 332, 148559 (October 2025)

Nandhu Varshini Gnanasekar a , Shanmugavelayutham Gurusamy a , Divyakaaviri Subramani b , Shankar Ramasamy b

107. Computational Insights into Graphene/WS₂ van der Waals Heterostructure as a Potential Sensor for Airborne Environmental Pollutants via First-Principles Calculations

Physica B: Condensed Matter, Volume 714, Pages 417501 (June 2025)

Deepak Arumugam, Subhalatha Shanmugam, Akilesh Muralidharan, Shankar Ramasamy

106. DESIGN AND SYNTHESIS OF 8-NITROQUINOLINE AZINE D-?-A MODULE CHEMOSENSORS: FLUOROGENIC ONSITE DETECTION OF SARIN GAS MIMIC-DCP

Talanta Open, Volume 12, Pages 100508 (June 2025)

Sentamil Selvi Ramasamy, Kaviyarasu Adhigaman, Vandana Nandakumar, Akilesh Muralidharan, Shankar Ramasamy, Suresh Thangaraj

105. Electrochemical Enhancement of Copper in a Nickel–Iron Layered Double Hydroxide Catalyst for Alkaline Oxygen Evolution Reactions

Inorganic Chemistry, Volume 64, Issue 22, page 10879–10893 (May 2025)

ayachandran Madhavan, Deepak Arumugam, Pavithra Karthikesan, Harshini Sharan, Shankar Ramasamy, Sajan Raj Sasirajan Littleflower, Alagiri Mani

104. Electrodeposited CoP₂ on CO₂-laser-modified graphite felt: a robust electrocatalyst for nitrite reduction to ammonia

Journal of Materials Chemistry A (April 2025)

Chae Eun Park, Rahul Kerkar, Deepak Arumugam, Jayaraman Theerthagiri, Shankar Ramasamy, Myong Yong Choi

103. Delineating the multifunctional performance of Janus WSSe with nonmetals in water splitting and hydrogen fuel cell applications via first-principles calculations

Physical Chemistry Chemical Physics, Volume 27, Issue 20, Pages 10826-10837 (April 2025)

Deepak Arumugam, Divyakaaviri Subramani, Shamini Pazhani Beena, Shankar Ramasamy

102. Design, Synthesis, and Evaluation of Nitroquinoline Fused Thiosemicarbazones for Anti-Cancer Activity on Human Cervical Cancer Cell Lines

ChemistrySelect, Volume 10, Issue 15, Pages e202405057 (April 2025)

Vandana Nandakumar, Sentamil Selvi Ramasamy, Kaviyarasu Adhigaman, Amsaveni Sundarasamy, Deepak Arumugam, Shankar Ramasamy, Raju Vivek, Suresh Thangaraj

101. Investigating the Antiproliferative Activity of Novel 4-Chloro-8-Nitro-1, 2-Dihydro-3-Quinoline Acylhydrazones on Human Cervical Cancer Cell Lines

Chemistry & Biodiversity, Volume 22, Issue 3, Pages e202401636 (March 2025)

Vandana Nandakumar, Sentamil Selvi Ramasamy, Kaviyarasu Adhigaman, Deepak Arumugam, Shankar Ramasamy, Raju Vivek, Shunmuganarayanan Athimoolam, Suresh Thangaraj



100. Benzothiazole-based Schiff base for sensing Ca²⁺ ions: Synthesis, DFT studies, toxicity evaluation in zebrafish embryo and in silico analysis of MMP-9 inhibition

Journal of Photochemistry and Photobiology A: Chemistry Volume 458, Pages 115985 (January 2025)
G. Sathiyaraj , M. Akilesh , A. Vignesh , K. Naveen Kumar , S. Gopinath, S. Mohanapriya , J.M. Malecki , K. Kadirvelu , R. Shankar, N. Dharmaraj

99. Exploration of thiosemicarbazone-quinolone hybrids over in-silico, antioxidant, and zebrafish embryo toxicity studies

Journal of Molecular Structure, Volume 1319, Pages 139513 (January 2025)
Kaviyarasu Adhiyaman, Vandana Nandakumar, Amsaveni Sundarasamy, Sentamil Selvi Ramasamy, Selvaraj Shyamsivappan, M. Saravanakumar, Srinivasan Palaniselvam, Saravanan Ramachandran, Deepak Arumugam, Shankar Ramasamy, Suresh Thangaraj

98. Exploring the Electrocatalytic Performance of Silicene and Single Atom Doped Silicene for HER, OER and ORR Activity Using Density Functional Theory

Chemical Physics Impact, Volume 9, Pages 100664 (December 2024)
Deepak Arumugam, Jaya Priya Sivakumar, Akilesh Muralidharan, Shankar Ramasamy

97. Demystifying Synergistic Multifunctional Electrocatalysis of N-Doped Graphene/WS₂ Heterostructure with Single-Atom Catalysts for Water Splitting and Fuel Cells

ACS Applied Materials & Interfaces (November 2024)
Deepak Arumugam, Divyakaaviri Subramani, Akilesh Muralidharan, Shankar Ramasamy

96. Investigating the Antiproliferative Activity of Novel 4-Chloro-8-Nitro-1,2-Dihydro-3-Quinoline Acylhydrazones on Human Cervical Cancer Cell Lines

Chemistry & Biodiversity (November 2024)
Vandana Nandakumar, Sentamil Selvi Ramasamy, Kaviyarasu Adhigaman, Deepak Arumugam, Shankar Ramasamy, Vivek Raju Athimoolam Shunmuganarayanan, Suresh Thangaraj

95. Sulfurization of Ternary NiCoZn Layered Double Hydroxides for Enhanced and Durable Alkaline Overall Water Splitting

Surfaces and Interfaces, Page 105485 (November 2024)
Jayachandran Madhavan a , Deepak Arumugam b , Harshini Sharan a , Pavithra Karthikesan a , Shankar Ramasamy b , Alagiri Mani

94. Exploring the fascinating interplay of epigenetically modified DNA bases with two dimensional bare and P-doped Si₂BN and BN sheets for biosensing applications: A compelling DFT perspective

International Journal of Biological Macromolecules, Pages 137032 (October 2024)
Akilesh Muralidharan , Divyakaaviri Subramani , Deepak Arumugam , Shamini Pazhani Beena , Shankar Ramasamy

93. Interfacial charge transfer modulation in laser-synthesized catalysts for efficient oxygen evolution

Journal of Materials Chemistry A, Volume 12, Issue 44, Pages 30269-30278 (October 2024)
Dong Hyeon Lee, Rahul Kerkar, Deepak Arumugam, Jayaraman Theerthagiri, Shankar Ramasamy, Soorathep Kheawhom, Myong Yong Choi

92. Unveiling the structure-property relationships of bimetallic nickel molybdenum metal organic framework for pseudocapacitor electrode materials: A combined approach of ...

Chemical Engineering Journal, Volume 495, Pages 153691 (September 2024)
Sureka Kanthasamy, Mohanapriya Subramani, Shankar Ramasamy, Selvaraju Thangavelu

91. Elucidating the hydrogen adsorption mechanism in bare and TMs (Ni, Pd and Cd) decorated Al₁₂P₁₂, B₁₂P₁₂ and C₂₄ nanocages for hydrogen storage via DFT study

International Journal of Hydrogen Energy, Volume 82, Pages 1351-1371 (September 2024)
Divyakaaviri Subramani, Deepak Arumugam, Akilesh Muralidharan, Shankar Ramasamy

90. Fluorophore-quencher complexes (Cu²⁺/Al³⁺) of coumarin Schiff bases as chemosensors for the detection of L-glutamic acid and L-arginine: in vitro and in vivo studies

Dalton Transactions, Volume 53, Issue 41, Pages 16941-16955 (September 2024)
M Ranjani, GA Thiruppathi, V Keerthana, M Ramya, P Kalaivani, S Selvakumar, R Shankar, K Srinivasan, P Sundararaj, R Prabhakaran



89. Intraphase Switching of Hollow CoCuFe Nanocubes for Efficient Electrochemical Nitrite Reduction to Ammonia

ACS Applied Materials & Interfaces, (August 2024)

Ahreum Min, Jueun Park, Talshyn Begildayeva, Jayaraman Theerthagiri, Deepak Arumugam, Cheol Joo Moon, Shankar Ramasamy, Myong Yong Choi

88. Nitroquinolone Fused Salicyl and Naphthyl Hydrazone Fluorescent Probes for the Detection of Fe³⁺ and Pb²⁺ Ions

Journal of Fluorescence, Pages 1-14 (July 2024)

Vandana Nandakumar, Sentamil Selvi Ramasamy, Kaviyarasu Adhigaman, Narmatha Ganesan, Divyakaaviri Subramani, Shankar Ramasamy, Raju Nandhakumar, Suresh Thangaraj

87. Unraveling the potential of transition metals as single atom catalyst in Graphene/WS₂ van der Waals heterostructure for enhanced HER performance—A first principles study

International Journal of Hydrogen Energy, Volume 68, Pages 545-558 (May 2024)

Deepak Arumugam, Mohanapriya Subramani, Divyakaaviri Subramani, Shankar Ramasamy

86. Atomic insights into the fluorinated pristine and defected graphene sheets for inducing the electronic and magnetic properties with the aid of scandium metal decoration—Acumen ...

Journal of Magnetism and Magnetic Materials, Volume 587, Pages 171263 (December 2023)

Divyakaaviri Subramani, Mohanapriya Subramani, Akilesh Muralidharan, Shankar Ramasamy

85. Theoretical aspects of the adsorption of normal and modified base pairs of DNA on graphene models toward DNA sequencing

Journal of Biomolecular Structure and Dynamics, Pages 1-15 (November 2023)

R Radhika, R Shankar

84. Theoretical insights on the development of a 55–77 graphene sheet by embedding Ag_n= 1-4 and Pd_n= 1-4 metal nanoclusters for efficient CO₂ capture

Journal of Molecular Graphics and Modelling, Volume 124, Pages 108573 (November 2023)

Mohanapriya Subramani, Vinnarasi Saravanan, Akilesh Muralidharan, Ravichandran Durai, Shankar Ramasamy

83. Probing the influence of defects and Si-doping in graphene sheet as an efficacious carrier for drug delivery system in gas and aqua phases—Combined DFT and classical MD simulation

Journal of Physics and Chemistry of Solids, Volume 181, Pages 111562 (October 2023)

Deepak Arumugam, Mohanapriya Subramani, Ravichandran Durai, Anitha Sambasivam, Shankar Ramasamy

82. Inquest for the interaction of canonical and non-canonical DNA/RNA bases with ternary based 2D Si₂BN and doped Si₂BN for biosensing applications

Journal of Biomolecular Structure and Dynamics, Pages 1-32 (October 2023)

Akilesh Muralidharan, Mohanapriya Subramani, Divyakaaviri Subramani, Shankar Ramasamy

81. Atomistic and molecular level portrayal of DNA–1, 8-naphthalimide interaction

Molecular Simulation, Volume 49, Pages 1542-1551 (September 2023)

R Radhika, R Shankar

80. Unpredicted coordination of hydrogen chloride in organoruthenium (II) pyrazolone complex: Synthesis, spectral and structural characterization

Inorganic Chemistry Communications, Volume 153, Pages 110849 (July 2023)

S Dharani, G Kalaiarasi, Vincent M Lynch, R Shankar, R Prabhakaran

79. Mitigation of indoor pollutants using 2D materials for enrichment of indoor environmental quality and human health: a review

Current Opinion in Environmental Science & Health, Volume 33, Pages 100460 (June 2023)

Mohanapriya Subramani, Akilesh Muralidharan, Deepak Arumugam, Akilan Rajamani, Shankar Ramasamy



78. Revealing the interfacial phenomenon of metal-hydride formation and spillover effect on C48H16 sheet by platinum metal catalyst (Pt (n= 1-4)) for hydrogen storage enhancement

International Journal of Hydrogen Energy, Volume 48, Pages 4016-4034 (February 2023)
Mohanapriya Subramani, Deepak Arumugam, Shankar Ramasam

77. Coumarin-Picolinohydrazone derived Schiff base as fluorescent sensor (OFF-ON) for detection of Al³⁺ ion: Synthesis, Spectral and theoretical studies

Journal of Molecular Structure, Volume 1273, Pages 134329 (February 2023)
D Ravichandran, M Ranjani, G Prabu Sankar, R Shankar, M Karthi, S Selvakumar, R Prabhakaran

76. Optoelectronic properties of hollow spheroid (ZnO) m quantum dots with nanotube (carbon and ZnO) nanocomposites in the solvent phase–A DFT/TD-DFT study

Materials Science and Engineering: B, Volume 287, Pages 116129 (January 2023)
S Gopalakrishnan, R Shankar, T Pazhanivel, M Priyadharshini, T Maiyalagan

75. Evidence of charge donation through synergistic effect of bioconjugated silver nanoparticles with flavanols accomplishing augmented antimicrobial and antioxidant activities

Journal of Molecular Liquids, Volume 368, Pages 120754 (December 2022)
S Anitha, R Selvapriya, R Shankar, B Nalini, V Sasirekha, J Mayandi

74. Probing of sequential atmospheric degradation of chlorine radical initiated 1, 8-cineole in the presence of O₂ and NO radical with the emission of secondary pollution

Environmental Pollution, Volume 300, Pages 118974 (May 2022)
Vasuki Tamilvanan, Mohanapriya Subramani, Divyakaaviri Subramani, Shankar Ramasamy

73. IDF21-0191 Plumbagin and Plumbagin amino acid ester conjugates inhibit amylin priori and post-priori

Diabetes Research and Clinical Practice, Volume 186 (April 2022)
V Narayanan, C Loganathan, M Kumarasamy, S Vasudevan, S Ramasamy, P Thayumanavan

72. Impact of Au¹⁴⁴ metal clusters on the structural and inhibitory mechanism of A β 42 peptide: a theoretical approach

Environmental Research, Volume 204, Pages 111920 (March 2022)
Vasudevan Saranya, Ramasamy Shankar, Mansour K Gatasheh, Sadaf Zehra

71. Reinforcing the tetracene-based two-dimensional C48H16 sheet by decorating the Li, Na, and K atoms for hydrogen storage and environmental application–A DFT study

Environmental Research, Volume 204, Pages 112114 (March 2022)
Mohanapriya Subramani, Akilan Rajamani, Vijayakumar Subramaniam, Mohammad Rafe Hatshan, Sivalingam Gopi, Shankar Ramasamy

70. Structural exploration of interactions of (+) catechin and (?) epicatechin with bovine serum albumin: Insights from molecular dynamics and spectroscopic methods

Journal of Molecular Liquids, Volume 348, Pages 118026 (February 2022)
S Anitha, V Saranya, R Shankar, V Sasirekha

69. ZnS quantum dots and Bi metals embedded with two dimensional γ -Bi₂O₄ nanosheets for efficient UV-visible light driven photocatalysis

Materials Research Bulletin, Volume 142, Pages 111387 (October 2021)
G Palanisamy, K Bhuvaneswari, T Pazhanivel, R Shankar, Khadijah Mohammedsleh Katubi, Norah Salem Alsaiari, Mohamed Ouladsmame

68. Effect of doping on the opto-electronic properties of hollow spheroid ZnO quantum dots: A theoretical study

Materials Science and Engineering: B, Volume 270, Pages 115220 (August 2021)
Sankarasubramanian Gopalakrishnan, Ramasamy Shankar, Ponmalai Kolandaivel



67. Polyyne-metal complexes for use in molecular wire applications: A DFT insight

Computational and Theoretical Chemistry, Volume 1202, Pages 113328 (August 2021)
AbhayRam Balakrishnan, R Shankar, S Vijayakumar

66. Tuning the reactivity of tri-s-triazine, trinitro-tri-s-triazine and ternary tri-s-triazine graphitic C₃N₄ quantum dots through H-functionalized and B-doped complexes: A ...

Chemosphere, Volume 272, Pages 129901 (June 2021)
D Ravichandran, R Akilan, S Vinnarasi, R Shankar, Sivakumar Manickam

65. Epigenetically modified nucleobases (5hmc, 5fc, and 5caC) interaction with boron and nitrogen doped porous graphene (B/N-pGr) as promising materials for biosensing application ...

Environmental Research, Volume 197, Pages 11133 (June 2021)
Vinnarasi Saravanan, Akilan Rajamani, Shankar Ramasamy, Alaa Baazeem, Indra Raj Upadhyaya

64. A first principle study of heme molecule as an active adsorbent for halogenated hydrocarbons

Journal of Molecular Modeling, Volume 27, Pages 209 (June 2021)
Rahul Suresh, VS Anithaa, R Shankar, Vijayakumar Subramaniam

63. A comprehensive experimental and computational study of highly efficient organic NLO crystal: Anilinium-L-Tartrate

Optics & Laser Technology, Volume 137, Pages 106800 (May 2021)
N Sudha, R Mathammal, R Shankar, G Sharon Benita

62. Kinetics and degradation of camphene with OH radicals and its subsequent fate under the atmospheric O₂ and NO radicals-A theoretical study

Chemosphere, Volume 267, Pages 129250 (March 2021)
Mohanapriya Subramani, Vinnarasi Saravanan, Jayaraman Theerthagiri, Vijayakumar Subramaniam, Thangavelu Pazhanivel, Shankar Ramasamy, Sivakumar Manickam

61. Enhanced thermoelectric performance of band structure engineered GeSe_{1-x}Te_x alloys

Sustainable Energy & Fuels, Volume 5, Pages 1734-1746 (February 2021)
D Sidharth, AS Alagar Nedunchezian, R Akilan, Anup Srivastava, Bhuvanesh Srinivasan, P Immanuel, R Rajkumar, N Yalini Devi, M Arivanandhan, Chia-Jyi Liu, G Anbalagan, R Shankar, R Jayavel

60. Functionalized oligoynes: comparison of theoretical parameters with experimental single molecule conductance

Structural Chemistry, Volume 32, Pages 1795-1806 (February 2021)
AbhayRam Balakrishnan, R Shankar, S Vijayakumar

59. Structural and electronic properties of graphene and its derivatives physisorbed by ionic liquids

Diamond and Related Materials, Volume 109, Pages 108005 (November 2020)
VS Anithaa, R Shankar, S Vijayakumar

58. Adsorption of H₂ and CO₂ gas molecules on Li/Na decorated Si₂BN nano-sheet for energy harvesting applications—A density functional study

Materials Letters, Volume 279, Pages 128487 (November 2020)
R Akilan, D Ravichandran, S Vinnarasi, R Shankar

57. Kinetics and degradation mechanism of atmospheric isoprene (2-methyl-2-butadiene (C₅H₈)) with chlorine radical and its derivatives—A theoretical study

International Journal of Quantum Chemistry, Volume 121, Pages e26573 (November 2020)
Mohanapriya Subramani, Akilan Rajamani, Ramasamy Shankar

56. Exploring two-dimensional graphene and boron-nitride as potential nanocarriers for cytarabine and clofarabine anti-cancer drugs

Computational Biology and Chemistry, Volume 88, Pages 107334 (October 2020)
Vinnarasi Saravanan, Akilan Rajamani, Mohanapriya Subramani, Shankar Ramasamy



55. Novel phenyl and thiophene dispiro indenoquinoxaline pyrrolidine quinolones induced apoptosis via G1/S and G2/M phase cell cycle arrest in MCF-7 cells

New Journal of Chemistry, Volume 44, Pages 15031-15045 (August 2020)

Selvaraj Shyamsivappan, Arjunan Saravanan, Raju Vivek, Thangaraj Suresh, Ramasamy Shankar, KM Gothandam, Palathurai Subramaniam Mohan

54. The hazardous effects of the environmental toxic gases on amyloid beta-peptide aggregation: A theoretical perspective

Biophysical Chemistry, Volume 263, Pages 106394 (August 2020)

Vasudevan Saranya, Pitchumani Violet Mary, Subramaniam Vijayakumar, Ramasamy Shankar

53. Adsorption of H₂ molecules on B/N-doped defected graphene sheets—a DFT study

Structural Chemistry, Volume 31, Pages 2413-2434 (July 2020)

Rajamani Akilan, Saravanan Vinnarasi, Subramani Mohanapriya, Ramasamy Shankar

52. In silico studies of the inhibition mechanism of dengue with papain

Journal of Biomolecular Structure and Dynamics, Volume 39, Pages 1912-1927 (April 2020)

Vasudevan Saranya, Ramachandran Radhika, Ramasamy Shankar, Subramaniam Vijayakumar

51. Exploring the synergistic effect of Ni x Sn 2x S 4x thiospinel with MWCNTs for enhanced performance in dye-sensitized solar cells, the hydrogen evolution reaction, and ...

Dalton transactions, Volume 49, Pages 5336-5351 (March 2020)

T Saravanakumar, T Selvaraju, KB Bhojanaa, M Ramesh, A Pandikumar, R Akilan, R Shankar, SJ Sardhar Basha

50. Exploring the nature of interaction and stability between DNA/RNA base pairs and defective & defect-dopant graphene sheets. A possible insights on DNA/RNA sequencing

International journal of biological macromolecules, Volume 146, Pages 387-404 (March 2020)

Vinnarasi Saravanan, Akilan Rajamani, Saranya Vasudevan, Shankar Ramasamy

49. Synthesis of self-assembled micro/nano structured manganese carbonate for high performance, long lifespan asymmetric supercapacitors and investigation of atomic-level ...

Journal of Energy Storage, Volume 27, Pages 101138 (February 2020)

M Karuppaiah, R Akilan, P Sakthivel, S Asaithambi, R Shankar, R Yuvakkumar, Y Hayakawa, GJJoES Ravi

48. Reconnoitring the nature of interaction and effect of electric field on Pd/Pt/Ni decorated 5-8-5/55-77 defected graphene sheet for hydrogen storage

International Journal of Hydrogen Energy, Volume 45, Pages 744-763 (January 2020)

R Akilan, S Vinnarasi, S Mohanapriya, R Shankar

47. Ab initio studies of adsorption of Haloarenes on Heme group

Journal of Molecular Modeling, Volume 26, Pages, 1-25 (December 2019)

Rahul Suresh, R Shankar, S Vijayakumar

46. Interaction of (G₄)₂ and (X₄)₂ DNA quadruplexes with Cu⁺, Ag⁺ and Au⁺ metal cations: a quantum chemical calculation on structural, energetic and electronic ...

Structural Chemistry, Volume 31, Pages 465-484 (September 2019)

Vinnarasi Saravanan, Akilan Rajamani, Vijayakumar Subramaniam, Shankar Ramasamy

45. Modeling of Si-B-N Sheets and Derivatives as a Potential Sorbent Material for the Adsorption of Li⁺ Ion and CO₂ Gas Molecule

ACS omega, Volume 4, Pages 13808-13823 (August 2019)

Akilan Rajamani, Vinnarasi Saravanan, Subramaniam Vijayakumar, Ramasamy Shankar

44. Coumarin based hydrazone as an ICT-based fluorescence chemosensor for the detection of Cu²⁺ ions and the application in HeLa cells

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, Volume 214, Pages 170-176 (May 2019)

Kailasam Saravana Mani, Ramar Rajamanikandan, Balasubramanian Murugesapandian, Ramasamy Shankar, Gandhi Sivaraman, Malaichamy Ilanchelian, Subramaniam Parameswaran Rajendran



43. Tetranuclear Palladacycles of 3-Acetyl-7-methoxy-2H-chromen-2-one Derived Schiff Bases: Efficient Catalysts for Suzuki–Miyaura Coupling in an Aqueous Medium

Inorganic Chemistry, Volume 58, Pages 8045-8055 (May 2019)
Sivadasan Dharani, Giriraj Kalaiarasi, Dharmalingam Sindhuja, Vincent M Lynch, Ramasamy Shankar, Ramasamy Karvembu, Rathinasabapathi Prabhakaran

42. DFT approach on stability and conductance of nine different polyene and cumulene molecules

Molecular Physics, Volume 118, Pages e1601785 (April 2019)
AbhayRam Balakrishnan, R Shankar, S Vijayakumar

41. Insights into structural and inhibitory mechanisms of low pH-induced conformational change of influenza HA2 protein: a computational approach

Journal of Molecular Modeling, Volume 25, Pages 1-14 (March 2019)
S Kannan, R Shankar, P Koldaivel

40. Mechanistic insights into the inhibition mechanism of cysteine cathepsins by chalcone-based inhibitors—a QM cluster model approach

Structural Chemistry, Volume 30, Pages 1779-1793 (March 2019)
C Pitchumani Violet Mary, R Shankar, S Vijayakumar

39. Theoretical insights into the metal chelating and antimicrobial properties of the chalcone based Schiff bases

Molecular Simulation, Volume 45, Pages 636-645 (February 2019)
C Pitchumani Violet Mary, R Shankar, S Vijayakumar

38. Structural insights into the anti-cancer activity of quercetin on G-tetrad, mixed G-tetrad, and G-quadruplex DNA using quantum chemical and molecular dynamics simulations

Journal of Biomolecular Structure and Dynamics, Volume 38, Pages 317-339 (February 2019)
S Vinnarasi, R Radhika, S Vijayakumar, R Shankar

37. Modeling of 2-D hydrogen-edge capped defected & boron-doped defected graphene sheets for the adsorption of CO₂, SO₂ towards energy harvesting applications

Applied Surface Science, Volume 463, Pages 596-609 (January 2019)
R Akilan, M Malarkodi, S Vijayakumar, S Gopalakrishnan, R Shankar

36. Synthesis and X-ray study of dispiro 8-nitroquinolone analogues and their cytotoxic properties against human cervical cancer HeLa cells

MedChemComm, Volume 10, Pages 439-449 (January 2019)
Selvaraj Shyamsivappan, Raju Vivek, Arjunan Saravanan, Thangaraj Arasakumar, Gopalan Subashini, Thangaraj Suresh, Ramasamy Shankar, Palathurai Subramaniam Mohan

35. Inhibition mechanism of cathepsin B by curcumin molecule: a DFT study

Theoretical Chemistry Accounts, Volume 138, Pages 21 (January 2019)
C Pitchumani Violet Mary, S Vijayakumar, R Shankar

34. Reduced bond length alternation and helical molecular orbitals in donor and acceptor substituted linear carbon chains

Journal of Theoretical and Computational Chemistry, Volume 17, Pages 1850049 (December 2018)
AbhayRam Balakrishnan, R Shankar, S Vijayakumar

33. A versatile “on-off-on” quinoline pyrazoline hybrid for sequential detection of Cu²⁺ and S²⁻ ions towards bio imaging and tannery effluent monitoring

Inorganica Chimica Acta, Volume 483, Pages 173-179 (November 2018)
Gopalan Subashini, Arjunan Saravanan, Selvaraj Shyamsivappan, Thangaraj Arasakumar, Viswanathan Mahalingam, Ramasamy Shankar, Palathurai Subramaniam Mohan

32. Structural exploration of viral matrix protein 40 interaction with the transition metal ions (Ag⁺ and Cu²⁺)

Journal of Biomolecular Structure and Dynamics, Volume 37, Pages 2875-2896 (November 2018)
V Saranya, R Shankar, S Vijayakumar



31. D–A–D structured bis-acylhydrazone exhibiting aggregation-induced emission, mechanochromic luminescence, and AI (III) detection

The Journal of Organic Chemistry, Volume 83, Pages 10770-10775 (September 2018)

Kuppusamy Santhiya, Shovan K Sen, Ramalingam Natarajan, Ramasamy Shankar, Balasubramanian Murugesapandian

30. DFT/TD-DFT study on halogen doping and solvent contributions to the structural and optoelectronic properties of poly [3, 6-carbazole] and poly [indolo (3, 2-b)-carbazole]

Structural Chemistry, Volume 29, Pages 1775-1796 (July 2018)

S Gopalakrishnan, S Vijayakumar, R Shankar

29. DFT/TD-DFT study on the electronic and spectroscopic properties of hollow cubic and hollow spherical (ZnO) m quantum dots interacting with CO, NO₂ and ...

Applied Physics A, Volume 124, Pages 1-13 (February 2018)

Sankarasubramanian Gopalakrishnan, Ramasamy Shankar, Ponmalai Kolandaivel

28. Metal chelating ability and antioxidant properties of Curcumin-metal complexes–A DFT approach

Journal of Molecular Graphics and Modelling, Volume 79, Pages 1-14 (January 2018)

C Pitchumani Violet Mary, S Vijayakumar, R Shankar

27. Theoretical investigation on hydrogen bond interaction of diketo/keto-enol form uracil and thymine tautomers with intercalators

Journal of Molecular Modeling, Volume 23, Pages 1-16 (November 2017)

VS Anithaa, S Vijayakumar, M Sudha, R Shankar

26. Unpredicted formation of copper (ii) complexes containing 2-thiophen-2-yl-1-thiophen-2-ylmethyl-1 H-benzoimidazole and their most promising in vitro cytotoxicity in MCF-7 and ...

New Journal of Chemistry, Volume 41, Pages 8885-8898 (July 2017)

P Naveen, Ruchi Jain, P Kalaivani, R Shankar, F Dallemer, R Prabhakaran

25. DFT-based investigation on adsorption of methane on pristine and defected graphene

Structural Chemistry, Volume 28, Pages 1935-1952 (July 2017)

VS Anithaa, R Shankar, S Vijayakumar

24. Quinoline appended pyrazoline based Ni sensor and its application towards live cell imaging and environmental monitoring

Sensors and Actuators B: Chemical, Volume 243, Pages 549-556 (May 2017)

Gopalan Subashini, Ramasamy Shankar, Thangaraj Arasakumar, Palathurai Subramaniam Mohan

23. New pyrazolo-quinoline scaffold as a reversible colorimetric fluorescent probe for selective detection of Zn²⁺ ions and its imaging in live cells

Journal of Photochemistry and Photobiology A: Chemistry, Volume 341, Pages 136-145 (May 2017)

Gayathri Kasirajan, Velmurugan Krishnaswamy, Nandhakumar Raju, Malathi Mahalingam, Mathusalini Sadasivam, Mohan Palathurai Subramaniam, Shankar Ramasamy

22. Role of 6-Mercaptopurine in the potential therapeutic targets DNA base pairs and G-quadruplex DNA: insights from quantum chemical and molecular dynamics simulations

Journal of Biomolecular Structure and Dynamics, Volume 36, Pages 1369-1401 (May 2017)

R Radhika, R Shankar, S Vijayakumar, P Kolandaivel

21. Comparative theoretical and experimental study on novel tri-quinoline system and its anticancer studies

Journal of Molecular Structure, Volume 1134, Pages 770-780 (April 2017)

Kasirajan Gayathri, Ramachandran Radhika, Ramasamy Shankar, Mahalingam Malathi, Krishnaswamy Savithiri, Hazel A Sparkes, Judith AK Howard, Palathurai Subramaniam Mohan

20. Growth and spectral analysis of piperazinium L-tartrate salt: A combined experimental and theoretical approach

Journal of Molecular Structure, Volume 1131, Pages 87-96 (March 2017)

R Mathammal, N Sudha, R Shankar, M Rajaboopathi, S Janagi, B Prabavathi



19. Adsorption of Mn atom on pristine and defected graphene: a density functional theory study

Journal of molecular modeling, Volume 23, Pages 1-17 (March 2017)
VS Anithaa, R Shankar, S Vijayakumar

18. A theoretical study on the reaction mechanism and kinetics of allyl alcohol (CH₂ = CHCH₂OH) with ozone (O₃) in the atmosphere

Molecular Physics, Volume 115, Pages 895-911 (February 2017)
C Elakiya, R Shankar, S Vijayakumar, P Kolandaivel

17. Theoretical studies on the interaction between the nitrile-based inhibitors and the catalytic triad of Cathepsin K

Journal of Biomolecular Structure and Dynamics, Volume 36, Pages 634-655 (February 2017)
C Pitchumani Violet Mary, R Shankar, S Vijayakumar

16. Novel Synthetic and Mechanistic Approach of TFA Catalysed Friedländer Synthesis of 2-Acylquinolines from Symmetrical and Unsymmetrical 1,2-Diketones with o-Aminoarylketones

ChemistrySelect, Volume 1, Pages 6823-6829 (December 2016)
Rajendran Satheeshkumar, Ramasamy Shankar, Werner Kaminsky, Karnam JayarampillaiRajendra Prasad

15. Interaction studies of human prion protein (HuPrP¹⁰⁹⁻¹¹¹: methionine-lysine-histidine) tripeptide model with transition metal cations

Journal of Molecular Graphics and Modelling, Volume 69, Pages 111-126 (September 2016)
C Pitchumani Violet Mary, R Shankar, S Vijayakumar, P Kolandaivel

14. Synthesis of first ever 4-quinolone-3-carboxylic acid-appended spirooxindole-pyrrolidine derivatives and their biological applications

Molecular diversity, Volume 21, Pages 37-52 (September 2016)
Thangaraj Arasakumar, Sadasivam Mathusalini, Athar Ata, Ramasamy Shankar, Subashini Gopalan, Krishnasamy Lakshmi, Pandiyarajan Sakthivel, Palathurai Subramaniam Mohan

13. Mechanism and kinetics of the atmospheric degradation of 2-formylcinnamaldehyde with O₃ and hydroxyl OH radicals – a theoretical study

Molecular Physics, Volume 114, Pages 3055-3075 (August 2016)
D Thangamani, R Shankar, S Vijayakumar, P Kolandaivel

12. Theoretical and experimental investigations on molecular structure of 7-Chloro-9-phenyl-2,3-dihydroacridin-4 (1H)-one with cytotoxic studies

Journal of Molecular Structure, Volume 1109, Pages 247-257 (April 2016)
Rajendran Satheeshkumar, Ramasamy Shankar, Werner Kaminsky, Sivalingam Kalaiselvi, Viswanadha Vijaya Padma, Karnam Jayarampillai Rajendra Prasad

11. Synthesis of bisbenzimidazo quinoline fluorescent receptor for Fe²⁺ ion in the aqueous medium—An experimental and theoretical approach

Journal of Molecular Structure, Volume 1099, Pages 257-265 (November 2015)
Malathi Mahalingam, Manikandan Irulappan, Gayathri Kasirajan, Mohan Palathurai Subramaniam, Shankar Ramasamy, Nusrath Unnisa

10. 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, Volume 41, Pages 633-652 (May 2014)
R Shankar, R Radhika, D Thangamani, L Senthil Kumar, P Kolandaivel

9. A strategic approach to the synthesis of novel class of dispiroheterocyclic derivatives through 1, 3 dipolar cycloaddition of azomethine ylide with (E)-3-arylidene-2, 3-dihydro ...

Tetrahedron Letters, Volume 54, Pages 3896-3901 (July 2013)
Kumarasamy Chandraprakash, Mathan Sankaran, Chokalingam Uvarani, Ramasamy Shankar, Athar Ata, Frederic Dallemer, Palathurai Subramaniam Mohan



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

Inorganica Chimica Acta, Volume 387, Pages 125-136 (May 2012)
R Shankar, P Kolandaivel

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

Journal of Physical Organic Chemistry, Volume 24, Pages 553-567 (October 2010)
R. Shankar, P. Kolandaivel, L. Senthilkumar

6. A theoretical study on decomposition and rearrangement reaction mechanism of trichloroacetyl chloride (CCl₃COCl)

International Journal of Quantum Chemistry, Volume 111, Pages 3482-3496 (October 2010)
R Shankar, P Kolandaivel, K Senthilkumar

5. Experimental and theoretical evaluation of dimerization mechanism in the synthesis of

7H-6,8-dichloro-7-methylpyrano[3,2-b:3,2-b']diquinoline

Journal of Molecular Structure, Volume 979, Pages 1-11 (August 2010)
Malathi Mahalingam a, Ramasamy Shankar b, Raymond J. Butcher c, Palathurai Subramaniam Mohan a, Ponmalaigounder Kolandaivel b

4. Reaction mechanism of cysteine proteases model compound HSH with diketone inhibitor

PhCOCOCH₃?nXn, (X = F, Cl, n = 0, 1, 2)

International Journal of Quantum Chemistry, Volume 110, Pages 1660-1674 (October 2009)
R. Shankar, P. Kolandaivel, K. Senthilkumar

3. Calculation of ionization potential and chemical hardness: A comparative study of different methods

International Journal of Quantum Chemistry, Volume 109, Pages 764-771 (October 2008)
R. Shankar, K. Senthilkumar, P. Kolandaivel

2. Reaction mechanism of O-acylhydroxamate with cysteine proteases

Journal of Chemical Sciences, Volume 119, Pages 533-544 (January 2008)
R. Shankar & P. Kolandaivel

1. Molecular Interaction of H₂, N₂, and HF Molecules with the Silicon Carbide (SiC) n=5-9 Clusters: A Theoretical Study

Journal of Computational and Theoretical Nanoscience, Volume 4, Number 4, pp. 787-796(10) (June 2007)
Shankar, R.; Kolandaivel, P.; Nirmala, V.; Narayandass, Sa. K.