

State University I "A++" Grade by NAAC I 26th Rank in MoE-NIRF Maruthamalai Road, Coimbatore, Tamil Nadu - 641 046.

Dr RAMASAMY SHANKAR

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Research Area

 2D Materials for Energy and Environmental **Applications**

• Degradation of Hazardous Atmospheric Reactions

Biomolecular interactions

Courses Teaching

- Classical Mechanics
- Quantum Mechanics
- Energy Resources
- Numerical Methods
- Statistical and Thermodynamics

Research Experience: 18 **Teaching Experience: 13**

Research Credentials (as on July 2024 – Source: Google scholar)

H-index: 1434 Citations: 21 i10-index: 42

Publications

International Journals: 107

Publications

International Journals - 107

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 CoP 2 on CO 2-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

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Dr RAMASAMY SHANKAR, Assistant Professor, Department of Physics

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: ChemistryVolume 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

ournal 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

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, Page105485 (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

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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 (Cu 2+/Al 3+) of coumarin Schiff bases as chemosensors for the

detection of I-glutamic acid and I-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+ lons

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 Agn= 1-4 and Pdn= 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 Ramasam

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

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81. Atomistic and molecular level portrayal of DNA-1, 8-napthalimide 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?42 peptide: a theoretical

approach

Environmental Research, Volume204, 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

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Dr RAMASAMY SHANKAR, Assistant Professor, Department of Physics

69. ZnS quantum dots and Bi metals embedded with two dimensional ?-Bi2O4 nanosheets for efficient UV-

visible light driven photocatalysis

Materials Research BulletinVolume142Pages111387 (October 2021)

G Palanisamy, K Bhuvaneswari, T Pazhanivel, R Shankar, Khadijah Mohammedsaleh Katubi, Norah Salem Alsaiari, Mohamed Ouladsmane

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

ny y no motar complexes for use in molecular wife applications. A St 1 molyne

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 Nedunchezhian, 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

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Dr RAMASAMY SHANKAR, Assistant Professor, Department of Physics

57. Kinetics and degradation mechanism of atmospheric isoprene (2?methyl?1, 3?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, Volume45, 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 ModelingVolume, 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

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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, Volume4, 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 polyyne 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 Kolandaivel

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, Volume45, 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, Pages21 (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

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Dr RAMASAMY SHANKAR, Assistant Professor, Department of Physics

33. A versatile "on-off-on" quinoline pyrazoline hybrid for sequential detection of Cu2+ and S? 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, Volume29, Pages 1775-1796 (July 2018)

S Gopalakrishnan, S Vijayakumar, R Shankar

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