Dr S VIJAYAKUMAR

Associate Professor & Head i/c
Department of Medical Physics

Bharathiar University

Tamil Nadu
E-mail: svijayakumar@buc.edu.in
Phone: 4222428546
Office Number: 0422-2428546

Research Area

- Weak Interactions
- Inhibiton mechanism of proteases
- Nano material

Courses Teaching

- Electronics and Instrumentation
- Atomic, Molecular, and Nuclear Physics
- Numerical and Computational techniques
- Electronics and Radiation Physics Lab

Research Experience:

Teaching Experience:

Research Credentials (as on August 2025 – Source: Google scholar)

H-index: 950 Citations: 17 i10-index: 29

Publications

International Journals: 64

Career

At Bharathiar University

1. Designation : Associate Professor
Period : February 2023 - Till Date

2. Designation : Assistant Professor
Period : February 2011 - February 2023

Education

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

M. Phil.
Subject : Physics
Institution : P S G College of Arts and Science
Affiliated University : Bharathiar University
Year of Award : April 2001

M. Sc.
Subject : Physics
Institution : P S G College of Arts and Science
Affiliated University : Bharathiar University
Year of Award : May 1999

B. Sc.
Subject : Physics
Institution : Gobi Arts and Science College
Affiliated University : Bharathiar University
Year of Award : May 1997

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Projects

National Level

Ongoing - completed - 1

0

Ongoing - completed - 2

Research Guidance

Completed

M.Phil. - 7 Ph.D. - 4

On Going

Ph.D. - 1

Programs organized

1. DST-PURSE Phase II sponsored "National Symposium on recent trends in Medical Physics" (2018-08-31 - 2018-08-30)

Visits

1. Visiting Fellow -)

Publications

International Journals - 64

64. Computational characterization of phytochemical inhibitors targeting cathepsin B for potential cancer therapy: A multi-parametric approach involving molecular docking, DFT and MD simulations study

Journal of Molecular Liquids 427 (2025) 127423 (June 2025)
M. Nandhini, Gopinath Samykannu, C. Pitchumani Violet Mary, S. Vijayakumar

63. Exploring novel nickel schiff-base complexes: One-pot green synthesis, density functional theory studies, and structural investigations toward energy storage applications

Journal of Power Sources 642 (2025) 236942 (June 2025)
S. Parveena, S. Balakrishnan, T. Premkumar, J. William, H. Nguyene, K. Srinivasan, S Vijayakumar, B. Abhayram, S. Govindarajan, T Ramkumar

62. Atomistic design of smart phosphorene nanocarriers for curcumin delivery: a DFT–MD study of doping and defect modulation

Structural Chemistry (2025) (June 2025)
M. Nandhini, Gopinath Samykannu & S. Vijayakumar

61. DFT Inquest on a 3d Transition Metal-Adsorbed Porphyrin Sheet for Spintronic and Optoelectronic Applications

ACS Appl. Electron. Mater. 7(8), 2025, 3201 - 3218 (April 2025)
Asnafarsin K A and Vijayakumar S

60. Structure based interaction and molecular dynamics studies of cysteine protease Cathepsin B against curcumin and resveratrol

Journal of Biomolecular Structure and Dynamics (2025) (November 2024)
M. Nandhini, C. Pitchumani Violet Mary, S. Gopinath & S. Vijayakumar

59. Structural and Electronic properties of Li adsorbed single and bilayer porphyrin sheets as an electrode material for energy storage devices – A DFT Analysis

Physical Chemistry Chemical Physics, 2024 (26) 7808 - 7820 (February 2024)
Asnafarsin K.A., Anithaa V. S., Abhayram Balakrishnan, Rahul Suresh, Norge Cruz Hernandez e and Vijayakumar S

58. Superatom molecular orbital in C80

Journal of computational chemistry 2024 (45) 827–833 (December 2023)
Padmavathy V, Artem V. Kuklin, Rahul Suresh, Vijayakumar S

57. Adsorption studies of dye molecule on two-dimensional assembly of porphyrin using density functional theory

Materials Physics and Chemistry 2023 (6) 1-8 (October 2023)
Rahul Suresh, R. Rajaramakrishna, S. Vijayakumar

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56. Santalol Isomers Inhibit Transthyretin Amyloidogenesis and Associated Pathologies in Caenorhabditis elegans

Frontiers in Pharmacology 924862, 13, (2022) 1-15 (June 2022)
A. Mohankumar, D. Kalaiselvi, G. Thiruppathi, S. Muthusaravanan4, S. Vijayakumar, R. Suresh, S. Tawat, P. Sundararaj

55. Adsorption of volatile organic compounds on pristine and defected nanographene

Computational and Theoretical Chemistry 1211, (2022) 113664 (May 2022)
VS Anithaa, R Suresh, AV Kuklin, S Vijayakumar

54. A density functional theory study on the water aggregation behaviour of fatty acid-based anionic surface active ionic liquids

Structural Chemistry 33 (3), (2022) 961-972 (March 2022)
S. Suresh, S. Vijayakumar

53. 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 204 (2023) 112114 (March 2022)
S. Mohanapriya, R. Akilan, S. Vijayakumar, Mohammad Rafe Hatshan, G. Sivalingam, R. Shankar

52. Structural and electronic properties of polyyne and cumulene chains with phenylene as central aromatic group: a density functional theory study

Structural Chemistry 33 (2), (2022) 511-526 (January 2022)
AR Balakrishnan, S Vijayakumar

51. Highly delocalised molecular orbitals in boron-, carbon-and nitrogen-based linear chains: A DFT study

Molecular Physics 120 (6), (2022) e2020923 (January 2022)
Highly delocalised molecular orbitals in boron-, carbon-and nitrogen-based linear chains: A DFT study

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

Computational and Theoretical Chemistry 1202 (2021) 1133328 (August 2021)
AbhayRam Balakrishnan, R. Shankar, S. Vijayakumar

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

Journal of Molecular Modeling (2021) 27: 209 (June 2021)
R.Suresh1 & V S Anithaa R Shankar S. Vijayakumar

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

Chemosphere 267 (2020) 129250 (March 2021)
S. Mohanapriya, S. Vinnarasi, T. Jayaraman, S. Vijayakumar, T. Pazhanivel, R. Shankar ,M. M. Sivakumar

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

Structural Chemistry 2021(32) 1795–1806 (February 2021)
AbhayRam Balakrishnan, R. Shankar & S. Vijayakumar

46. Computational study of metal ions adsorption on pristine and heteroatom doped peritetracene

Computational and Theoretical Chemistry 1191 (2020) 113006 (December 2020)
S. Sangavi, N. Santhanamoorthi, S. Vijayakumar

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

Diamond and related materials 109 (2020) 108005 1-14 (November 2020)
V.S.Anithaa, R.Shankar, S.Vijayakumar

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

Bio physical chemistry 2020 (263) 106394 (1-16) (August 2020)
V. Saranya, Pitchumani Violet Mary, S. Vijayakumar, R. Shankar

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43. Enhanced Li+ ion adsorption on pristine and defected graphene via organic radical interaction – A DFT study

Physica B: Physics of Condensed Matter 611 (2021) 412700 (1-11) (June 2020)
S. Sangavi, N. Santhanamoorthi, S. Vijayakumar

42. Molecular dynamics simulation involved in expounding the activation of adrenoceptors by sympathetic nervous system signaling

Structural Chemistry 2020 (31) 1869–1885 (May 2020)
Rahul Suresh & S. Vijayakumar

41. Quantum Chemical Support on the Two-Dimensional Assembly of Porphyrin Rings in the Application of Energy-Storage Devices

Journal of Physical Chemistry C (2020), 124, 9712 - 9723 (April 2020)
Rahul Suresh and S. Vijayakumar

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

Journal of Biomolecular Structure and Dynamics (2021) 39, NO. 6, 1912–1927 (April 2020)
V. Saranya, R.Radhika,R. Shankar &S. Vijayakumar

39. DFT study of adsorption of ions on doped and defective graphene

Materials Today Communications 2020 (22) 100714 (March 2020)
S. Sangavi,N. Santhanamoorthi, S. Vijayakumar

38. The effect of edge termination on Li+ ion adsorption of pristine and defected graphene sheets

Journal of Material Science (2020) 55: 5920 - 5937 (February 2020)
S. Sangavi, N. Santhanamoorthi, S. Vijayakumar

37. Adsorption of Greenhouse Gases on the Surface of Covalent Organic Framework of Porphyrin – An Ab Initio Study

Physica E: Low-dimensional Systems and Nanostructures 126 (2021) 114448 (1-14) (February 2020)
Rahul Suresh & S. Vijayakumar

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

Journal of Molecular Modeling (2020) 26: 6, 1- 25 (December 2019)
Rahul Suresh & R. Shankar & S. Vijayakumar

35. 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 properties

Structural Chemistry 2020 (31) 465 - 484 (September 2019)
S. Vinnarasi, R. Akilan, S. Vijayakumar, R. Shankar

34. 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 2019 4 (9), 13808-13823 (August 2019)
R. Akilan, S. Vinnarasi, S. Vijayakumar, R Shankar

33. DFT approach on stability and conductance of nine different polyyne and cumulene molecules

Molecular Physics 2020 (118) No.2 e1601785 (April 2019)
AbhayRam Balakrishnan, R. Shankar & S. Vijayakumar

32. Structure, stability and reactivity of neutral bimetallic manganese oxide clusters with CO and NO—a DFT study

Structural Chemistry 2019 (30) 2109 - 2122 (April 2019)
S. Suresh, S.Vijayakumar, P.Selvarengan

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

Structural Chemistry 2019 (30) 1779–1793 (March 2019)
C. Pitchumani Violet Mary, R. Shankar S. Vijayakumar

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

Molecular Simulation 2019 (45) 8, 636 - 645 (February 2019)
C. Pitchumani Violet Mary, R. Shankar S. Vijayakumar

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

Journal of Biomolecular Structure and Dynamics (2020) (38) 2 317 - 339 (February 2019)
S. Vinnarasi, R. Radhika, S. Vijayakumar & R. Shankar

28. 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 2019 (463) 1, 596 - 609 (January 2019)
R. Akilan, M. Malarkodi, S. Vijayakumar, S. Gopalakrishnan, R. Shankar

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

Theoretical Chemistry Accounts (2019) 138:21 1 - 16 (January 2019)
C. Pitchumani Violet Mary, S. Vijayakumar, R. Shankar

26. Reduced bond length alternation and helical molecular orbitals in Donor and Acceptor substituted linear carbon chains

Journal of Theoretical and Computational Chemistry 2018 (17) 08, 1850049 (December 2018)
AbhayRam Balakrishnan, R.Shankar, S. Vijayakumar

25. Structural exploration of Viral matrix protein 40 interaction with the transition metal ions (Ag and Cu)

Journal of Biomolecular Structure and Dynamics 2019 (37) 2875-2896 (November 2018)
V. Saranya, R. Shankar & S. Vijayakumar

24. Density functional theory study on the adsorption of alkali metal ions with pristine and defected graphene sheet

Molecular Physics 2019 (117) 4, 462 - 473 (September 2018)
S. Sangavi, N. Santhanamoorthi & S. Vijayakumar

23. Effect of side chain edge functionalization in pristine and defected graphene- DFT study

Computational and Theoretical Chemistry 2018 (1135) 34–47 (July 2018)
V. S. Anithaa, and Vijayakumar S

22. 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 2018 (29) 6, 1775 - 1796 (July 2018)
S. Gopalakrishnan, S. Vijayakumar, R. Shankar

21. Electronic and optical properties of edge modified peritetracene: a DFT study

Structural Chemistry 2018 (29) 6, 1853 - 1865 (July 2018)
S. Sangavi, N. Santhanamoorthi, S. Vijayakumar

20. Impact of Oxygen Functional Groups on Reduced Graphene Oxide- Based Sensors for Ammonia and Toluene Detection at Room Temperature

ACS Omega 2018 (3) 4105 - 4112 (April 2018)
C. R. Minitha, V. S. Anithaa, Vijayakumar S., and R. T. Rajendra Kumar

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

Journal of Molecular Graphics and Modelling 2018 (79) 1 - 14 (January 2018)
C. Pitchumani Violet Mary, R. Shankar, and S. Vijayakumar

18. Magnetite Nanoparticle Decorated Reduced Graphene Oxide Composite as an Efficient and Recoverable Adsorbent for the Removal of Cesium and Strontium Ions

Industrial and Engineering Chemical Research 2018 (57) 1225 - 1232 (January 2018)
C. R. Minitha, Rahul Suresh, Ujjwal Kumar Maity, Yuvaraj Haldorai, Vijayakumar S, Periasamy Manoravi, Mathew Joseph,and R. T. Rajendra Kumar

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

Journal of Molecular Modeling 2017 (23) 333, 1 - 16 (November 2017)
Anithaa V S, Vijayakumar S, Sudha M and Shankar R

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

Structural Chemistry 2017 (28) 1935 - 1952 (July 2017)
V. S. Anithaa1 R. Shankar and S. Vijayakumar

15. Role of 6-Mercaptopurine in the potentialtherapeutic targets DNA base pairs and Gquadruplex DNA: insights from quantum chemical and molecular dynamics simulations

Journal of Biomolecular Structure and Dynamics 2018 (36) 1369 - 1401 (May 2017)
R. Radhika, R. Shankar, S. Vijayakumar and P. Kolandaivel

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

Journal of Molecular Modeling 2017 (23) 132, 1 - 17 (March 2017)
V. S. Anitha R. Shankar and S. Vijayakumar

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

Molecular Physics 2017 (115) ,7, 895 - 911 (February 2017)
C. Elakiya, R. Shankar, S. Vijayakumar and P. Kolandaivel

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

Journal of Biomolecular Structure and Dynamics 2018 (36),634 - 655 (February 2017)
C. Pitchumani Violet Mary, R. Shankar & S. Vijayakumar

11. Interaction studies of human prion protein (HuPrP109–111:methionine-lysine-histidine) tripeptide model with transition metalcations

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

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

Molecular Physics 2016 (114) , 20, 3055 - 3075 (August 2016)
D. Thangamani, R. Shankar, S. Vijayakumar & P. Kolandaivel

9. From Catalytic Mechanism to Rational Design of Reversible Covalent Inhibitors of Serine and Cysteine Hydrolases

Israel Journal of Chemistry, 54 & 1137 - 1151 (May 2014)
M. Shokhen, M. Hirsch, N. Khazanov, R. Ozeri, N. Perlman, T. Traube, S. Vijayakumar, and A. Albeck

8. . Network of secondary-substituted adamantane amines

Journal of Physical Organic Chemistry, 26 &917–926 (September 2013)
A. Pandaa, S. Vijayakumar, D. J. Klein, and A. Ryzhov

7. Differentiating Serine and Cysteine Protease Mechanisms by New Covalent QSAR Descriptors

ChemBioChem 12 & 1023 – 1026 (March 2011)
M. Shokhen, T. Traube, S. Vijayakumar, M. Hirsch, N. Uritsky, and A. Albeck

6. EMBM – a New Enzyme Mechanism Based Method for Rational Design of Chemical Sites of Covalent Inhibitors

Journal of Chemical information and modeling 50 & 2256 - 2265 (November 2010)
T. Traube, S. Vijayakumar, M. Hirsch, N. Uritsky, M. Shokhen, and A. Albeck

5. Isomerization study of C5H5NO molecules

International Journal of Quantum Chemistry 107, 769 -781 (October 2006)
S. Vijayakumar, P. Kolandaivel

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4. Reaction Mechanism of HSH and CH3SH with NH2CH2COCH2X (X=F and Cl) molecules

International Journal of Quantum Chemistry 2008 (108) issue 5, 927 – 936 (October 2006)
S. Vijayakumar, P. Kolandaivel

3. Study of static dipole Polarizabilities, Dipole moments, and Chemical hardness for linear CH3-(C?C)n-X (n=1-4, X=H, F, Cl, Br, NO2) molecules

Journal of molecular structure (THEOCHEM) 770 & 23-30 (September 2006)
S. Vijayakumar, P. Kolandaivel

2. Isomerization of C3H3NO isomers. Ab initio study

Molecular Physics 104 & 1401 - 1411 (August 2006)
S. Vijayakumar, P. Kolandaivel

1. Red-shifted and improper blue-shifted hydrogen bonds in dimethyl ether (DME)n (n=1–4) and hydrated (DME)n (n=1–4) clusters. A theoretical study

Journal of molecular structure 734 & 157-169 (January 2005)
S. Vijayakumar, P. Kolandaivel

Projects

Completed - 3

1. Quantum chemical (QM) and quantum mechanics / molecular mechanics (QM/MM) studies of catalytic mechanism and inhibition of Cysteine proteases DST – SERB 19.9 lakhs (September 2013 - September 2016)

2. Investigation of opto-electronic properties of metallopolyynes for molecular wire applications.– BEICH research fellowship RUSA 2.0 - BEICH 7.0 lakhs (-)

3. Computational Investigation on enzymatic inhibition properties of phytochemical compounds against Cancer involving cysteine and matrix metalloproteinases RUSA 2.0 - BCTRC 7.88 lakhs (-)