A.Suvitha

Personal information

Permanent Address

5/498, Balaji Nagar, Adhavathur(east), Srirangam Taluk, Trichy-620102

Email suvithaa@gmail.com

Phone Number 8248432267

Nationality Indian

Caste Reddiyar

Marital status Married and two children

Date of Birth 15th September 1976

Career Objective To pursue dedicated teaching, research and management assignments in academic institution

Educational Qualification

Ph. D. in Chemistry [2001 - 2007]**,** Indian Institute of Technology Madras, Chennai - 600 036, India.

M. Sc. in Chemical sciences [1998 - 2000], Department of Chemistry, Pondicherry University, Pondicherry – 625 021, India.

B. Sc. in Chemistry [1995 - 1998], Gandhigram Rural Institute (Deemed University), Gandhigram, Dindugal – 641 046, India.

Research Experience(3 years)

2007 – 2010 – Post doctoral fellow Institute for Materials Research (IMR), Tohoku University, Sendai, Japan) Computational materials science

Aug. 2007 – Apr. 2009 – Structure based drug designing for controlled release of anticancer drugs and structural analysis of the drugs used in photodynamic therapy using computational tools

Apr. 2009 – Mar. 2010 - Impurity in the grain boundary of Pc –Silicon: Relevance to improve the Polycrystalline silicon material for solar cell.

April 2010 – September 2010 – Evaluation of boron compounds for hydrogen storage materials a solution to future fuel.

Teaching Experience- 14 years 4 months

August 2021 – till date – Associate Professor,Thassim Beevi Abdul Kader College for Women,Kilakarai

July 2014 – November 2020 – Assistant Professor Research, SASTRA Deemed University, and Thanjavur.

May 2013 – May 2014 – Assistant Professor, Ramco Institute of Technology, Rajapalayam.

August 2012 – May 2013 – Assistant Professor, Cauvery Engineering College, Trichy.

July 2001 – July 2007 – Teaching Assistant, Indian Institute of Technology, Madras, Chennai.

Research Interest

Synthesis of highercoordinate silicon compounds, transition metal complexes and nanoparticles that has relevance to biosilicification.

Computational chemistry for designing of materials for targeted drug delivery systems, catalytic, hydrogen storage and polycrystalline solar cell materials.

Fellowships/Honors

Qualified **GATE** (Graduate aptitude test in Engineering), 2000

Visiting professor , Tohoku University Sendai, 2018 – 2019

Computional Skills

TDDFT, Virtual screening of drug, Molecular dynamics simulation using gromacs. Quantum chemical calculations, Transport properties for molecular electronics, using Gaussian 03, VASP and ATK codes. Construction of grain boundary using GB studio. Visualizing tools - Material studio, Gauss view.

Funded Research Project

DST Fast track Young scientist award (Project No.CS038/2013) Entitled: Inclusion Complexes of Cisplatin and its Analogues - Drug release mechanism and its reactivity towards non-specific targets. - **Rs. 13, 58,000/- (2015 – 2018)**

DST –EMR Project –Co –PI Hydrogen Storage on alkali metal functionalized porous discrete organic and polymer hosts for on-board utilization **Rs. 23.95 lakhs (2015 – 2018)**

Research Collaborators

1. **Professor Y. Kawazoe**, Niche, Tohoku University, Sendai, Japan.
2. **Professor T. Masae,** Tohoku University, Sendai, Japan.
3. **Professor Nail J Wheate**, The University of Sydney, Australia.

Subjects Handled

Engineering Chemistry – B.Tech
Environmental Science - B.Tech
Inorganic chemistry – I & II -Chemistry of Main group elements – M.Sc Chemistry (Intg)
Cheminformatics – B.Tech Bioinformatics
Bioinorganic Chemistry – M.Sc Chemistry

Publications

1. Effect of water molecule in the structure, stability, and electronic properties of sulfur trioxide clusters: a computational analysis R. Sahara A. Suvitha, N. S. Venkataramanan Monatshefte für Chemie - Chemical Monthly 153, 347–357.
2. A computational study on the complexation of bisbenzimidazolyl derivatives with cucurbituril and cyclohexylcucurbituril Y Kawazoe N. S. Venkataramanan, A. Suvitha, R. Sahara Journal of Inclusion Phenomena and Macrocyclic Chemistry 100, 217-231
3. Intermolecular interactions in microhydrated ribonucleoside and deoxyribonucleoside: A computational study NS Venkataramanan, A Suvitha, R Sahara, Y Kawazoe Computational and Theoretical Chemistry 1204, 113422
4. Deciphering the nature of interactions in nandrolone/testosterone encapsulated cucurbituril complexes: a computational study, A. Suvitha, M Soussi, Ryoji Sahara; *Journal of Inclusion Phenomena and Macrocyclic Chemistry* **2019**, 93, 183-192.
5. A theoretical exploration of the intermolecular interactions between resveratrol and water: a DFT and AIM analysis, **A Suvitha**, N.S

Venkataramanan, R Sahara, Y. Kawazoe ; *Journal of Molecular Modeling* **2019**, 25, 56.

6. Unraveling the binding nature of hexane with quinone functionalized pillar [5] quinone: a computational study, N.S. Venkataramanan A. **Suvitha,** Y. Kawazoe; *Journal of Inclusion Phenomena and Macrocyclic Chemistry* **2019**, 95, 307-319.

7. Structure, stability, and nature of bonding between high energy water clusters confined inside cucurbituril: A computational study, N.S. Venkataramanan, **A. Suvitha**, Ryoji Sahara; *Computational and Theoretical Chemistry* **2019**, 1148, 44-54.

8. Unravelling the nature of binding of cubane and substituted cubanes within cucurbiturils: A DFT and NCI study N.S.Venkataramanan, A. **Suvitha,** Y. Kawazoe; *Journal of Molecular Liquids* **2018**, 260, 18-29.

9. Nature of bonding and cooperativity in linear DMSO clusters: A DFT, AIM and NCI analysis, N S Venkataramanan, **A Suvitha**; *Journal of Molecular Graphics and Modelling* **2018**, 81, 50-59.

10. Piperine Encapsulation within Cucurbit[n]uril (n=6,7): A Combined Experimental and Density Functional Study, B. Mohanty, **A Suvitha**, N.S. Venkataramanan; *Chemistry select* **2018**, 3, 1933-1941.

11. Density functional theory study on the dihydrogen bond cooperativity in the growth behavior of dimethyl sulfoxide clusters, N. S. Venkataramanan, **A. Suvitha**, Y. Kawazoe; *Journal of Molecular Liquids* **2018,** 249, 454–462.

12. Structure, electronic, inclusion complex formation behavior and spectral properties of pillarplex, N.S.Venkataramanan, **A. Suvitha**; *Journal of Inclusion Phenomena and Macrocyclic Chemistry* **2017**, 88, 53-67.

13. Trapping of organophosphorus chemical nerve agents by pillar[5]arene: A DFT, AIM, NCI and EDA analysis, **A. Suvitha,** N.S. Venkataramanan; *Journal of Inclusion Phenomena and Macrocyclic Chemistry* **2017**, 87, 207-218.

14. Structure, stability and reactivity of neutral and charged monomeric chromium oxide clusters, S.S. Nair, S. Prakash, D. Vignesh, **A. Suvitha,** N.S.

Venkataramanan; *Computational and Theoretical Chemistry* **2016**, 1082, 58-66.

15. Loading of a Phenanthroline-Based Platinum(ii) Complex onto the Surface of a Carbon Nanotube via π-π Stacking, S.A. Houston, N.S. Venkataramanan,
A. Suvitha, N.J. Wheate; *Australian Journal of Chemistry* **2016**, 69, 1124-1129.

16. NHC-Catalyzed Benzylic Csp^3–H Bond Activation of Alkylarenes and N- Benzylamines for the Synthesis of 3H-Quinazolin-4-ones: Experimental and Theoretical Study, A. Alanthadka, E.S. Devi, S. Nagarajan, **A. Suvitha,** C.U. Maheswari ; *European Journal of Organic Chemistry* **2016,** 28, 4872-4880.

17. Encapsulation of sulfur, oxygen, and nitrogen mustards by cucurbiturils: A DFT study, N.S. Venkataramanan, S. **Ambigapathy**; *Journal of Inclusion Phenomena and Macrocyclic Chemistry* **2015**, 83, 387-400.

18. Computational study on the interactions of mustard gas with cucurbituril macrocycles, N.S. Venkataramanan, **A. Suvitha,** H. Mizuseki, Y. Kawazoe, *International Journal of Quantum Chemistry* **2015**, 115, 1515-1525.

19. DFT calculations on polarizabilities and hyperpolarizabilities for the neutral and anionic yttrium oxide clusters, **A. Suvitha,** N.S. Venkataramanan, *Journal of Theoretical and Computational Chemistry* **2015**, 14, 1550049.

20. A Theoretical Study of the Effects of Transition Metal Dopant on the Adsorption and Dissociation of Hydrogen on Nickel Clusters, N.S. Venkataramanan, **A. Suvitha,** H. Mizuseki, Y.Kawazoe; *International Journal of Quantum Chemistry* **2013**,113, 1940 – 1948.

21. Theoretical Prediction of the Complexation Behaviors of Antitumor Platinum Drugs with Cucurbiturils, N.S. Venkataramanan, **A. Suvitha,** H. Mizuseki, Y. Kawazoe; *Journal of Physical Chemistry B* **2012**,116, 14029 – 14039.

22. Electronic Structures and Spectra of Symmetric Meso-Substituted Porphyrin: DFT and TDDFT—PCM Investigations, N.S. Venkataramanan, **A. Suvitha,** H. Nejo, H. Mizuseki, Y. Kawazoe; *International Journal of Quantum Chemistry* **2011**, 111, 2340-235.

23. First Principles Calculations on ∑3 Grain Boundary Impurities in Polycrystalline Silicon, **A. Suvitha,** N.S. Venkataramanan, R. Sahara, H. Mizuseki, Y. Kawazoe; *Japanese Journal of Applied Physics* **2010**, 49, 04DP02 (1-4).

24. A combined experimental and theoretical investigation on the oxygenation of organic sulfides by oxo(salen)chromium(V) ion, N.S. Venkataramanan, S. Rajagopal, **A. Suvitha,** Y. Kawazoe; *Journal of Physical Organic Chemistry* **2009**, 22, 650 - 660.

25. Theoretical Insights into the Formation, Structure, and Electronic properties of Anticancer Oxaliplatin Drug and Cucurbit[n]urils n = 5 to 8, **A. Suvitha**, N.S. Venkataramanan, H. Mizuseki, Y. Kawazoe; *Journal of Inclusion Phenomena Macrocyclic Chemistry* **2009**, 66, 213 - 218.

26. Structures of small YmAln clusters: A DFT study, N.S. Venkataramanan, **A. Suvitha,** R. Note, Y. Kawazoe; *Journal of Molecular Structure(THEOCHEM)*, **2009**, 902, 72-78.

27. TD-DFT studies on Hematoporphyrin and its Dimers, **A. Suvitha,** R.V. Belosludov, H. Mizuseki, Y. Kawazoe, M. Takeda, M. Kohno, N. Ohuchi; *Journal of the Japan institute of metal and materials*, **2009**, 73, 555-558.

28. TD-DFT studies on Hematoporphyrin and its Dimers, **A. Suvitha,** R.V. Belosludov, H. Mizuseki, Y. Kawazoe, M. Takeda, M. Kohno, N. Ohuchi; *Materials Transactions*, **2008**, 49, 2416-2419.

29. Effective synthesis of hexacoordinate silicates of 2,3-dihydroxynaphthalene under microwave condition and X - ray crystal structure of bis (tri-n-butylammonium)tris(2,3-dihydroxynaphthalato) silicate, **A. Suvitha**, B. Varghese, M. N. Sudheendra Rao, G. Sundararajan**,** B.Viswanathan, Indian *Journal of chemistry section .A: Inorganic & Physical, Theoretical & analytical* **2006**, 45A, 2193-2198.

30. **A. Suvitha,** B. Varghese, M.N.S. Rao, Bis(diisobutylammonium)tris(naphthalene-2,3-diolato)silicate acetonitrile trisolvate; *Acta Crystallographica Section E* **2006,** E62, o344-o346.

Workshop organized

1. One day workshop on computational chemistry and computational biology - 15th July 2018
2. Workshop on computational Materials Science – 15th and 16th November 2016

Books Chapters

1. Functionalized Nanofullerenes for Hydrogen Storage: A Theoretical Perspective" N.S. Venkataramanan, A. Suvitha, H. Mizuseki, Y. Kawazoe, in "Hand book on Fullerenes: Synthesis, Properties and Application" Robert F. Verner and Carlos Benvegnu Nova Publishers (2011) **ISB**