Name : Dr. S KARTHIKEYANAN
Designation with Department : Assistant Professor of Chemistry
KhadirMohideen College
Adirampattinam – 614 701
Age and Date of Birth : 48 years, 28-04-1973
Qualification : M.Sc., Ph. D.,

Course	UG	PG	Ph. D
Year	1996	1998	2006
College/ University	KhadirMohideen college, Adirampattinam	KhadirMohideen college, Adirampattinam	IIT Madras

Residential Address : 10/10 Mariamman kovil Street, Adirampattinam- 614701.
Phone Number : 9626790392
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Awards and Honors :

Teaching Experience : UG : 10
PG : 10
M. Phil : -

Research areas of interest:

- Theoretical Chemistry (computational) & Molecular spectroscopy
- Intermolecular interactions, molecular clusters containing π-systems and nanomaterial design.
- Dye Sensitized Solar Cells (DSSCs), Sensor, and Hydrogen storage

Guidance of M.Phil.and Ph.D.

M. Phil. Awarded : 02
Ph.D. Awarded :
Ph.D. thesis submitted :
Ph.D. Guiding :

Research Project :
Research Experience

Assistant Professor INDIA

Khadir Mohideen College (Affiliated to Bharathidasan University)

February 2018 – till now

Assistant Professor INDIA

Kalasalingam University (KLU)

June 2016 – February 2018

Postdoctoral Fellow,

SungKyunKwan University (SKKU) SOUTH KOREA

August 2012- August 2015 **(Prof. Jin Yong Lee)**

Postdoctoral Fellow,

Institute of Molecular Science (**IMS**)

April 2011- March 2012 (**Prof. Shigeru Nagase**) JAPAN

Postdoctoral Scientist,

Pohang University of Science and Technology

(**POSTECH**) March 2010- February 2011 SOUTH KOREA

(Prof. Kwang S. Kim, and Prof. Pavel Hobza)

Postdoctoral Scientist,

Pohang University of Science and Technology

(**POSTECH**) Period: March 2007- February 2010 SOUTH KOREA

(Prof. Kwang S. Kim)

Research Associate

Indian Institute of Technology, Madras

Period: 1st September 2006 – 26th February 2007 INDIA

(**Prof. K. Mangala Sunder)**

Visiting Scientist, Universitat of Stuttgart

Period: 1st February -31st July 2006 GERMANY

- Developed a theoretical method for calculating the rotational-vibrational energies of large molecules.
- Simulation of IR spectra of biomolecules.

Ph. D. IIT, Madras Department of Chemistry INDIA

Advisor: **Prof. K. Mangala Sunder**

Development of theoretical methods for studying and calculating the intensities of transitions between rotational-vibrational energy levels in polyatomic molecules, To this end a new analytic procedure has been developed for deriving effective Hamiltonians for

studying molecules exhibiting strong Coriolis coupling between one or many degrees of freedom**.**

Project Associate

Indian Institute of Technology, Madras

Period: 5th December 1998 – 31st December 2000 INDIA

(**Prof. K. Mangala Sunder)**

Details of Papers Published

H-index: 19

S. No.	Author, Title, Journal name, Volume, Page, Year	Impact factor
1	**S. Karthikeyan**, Mangala Sunder Krishnan and Tucker Carrington Jr., Calculating intensities using effective Hamiltonians in terms of Coriolis-adapted normal modes. *J. Chem. Phys*, **122**, 034106 (2005).	3.176
2	**S. Karthikeyan**, Theoretical investigation of the molecular structure and vibrational spectra of 2,4 cyclopendatiene-1-one, 2, 4-cyclopentadiene-1-thione and 2,4-cyclopentadiene-1-selenone, *Journal of Molecular Structure* (THEOCHEM), **813(1-3)**, 29 (2007).	1.602
3	**S. Karthikeyan**, J. N. Singh, and K. S. Kim, Undissociated versus Dissociated Structures for Water Clusters and Ammonia-Water clusters: (H2O)n and NH3(H2O)n-1 (n=5,8,9,21). Theoretical Study. *J. Phys. Chem. A*, **112**, 6527 (2008).	2.883
4	**S. Karthikeyan**, J. N. Singh, M. Park, and K. S. Kim, Structures, energetic, vibrational spectra of NH4+(H2O)n=4,6 clusters: Ab initio calculations and first principles molecular dynamics simulations. *J. Chem. Phys.*, **128**, 244304 (2008).	3.176
5	**S. Karthikeyan**, M. Park, I. Shin, and K. S. Kim, Structure, Stability, Thermodynamic Properties, and IR Spectra of the Protonated Water Octamer. *J. Phys. Chem. A*, **112**, 10120 (2008).	2.883
6	**S. Karthikeyan**, and K. S. Kim, Structure, Stability, Thermodynamic Properties, and IR Spectra of the Protonated Water Cluster H+(H2O)9. *Mol. Phys.*, **107(8-12)**, 1169 (2009).	1.839
7	J. Y. Park, Y. S. Lee, B. Y. Chang, **S. Karthikeyan**, K. S. Kim, B. H. Kim, S. M. Park, (R)-Lipo-Diaza-18-Crown-6 Self-Assembled monolayer as a selective	5.636

	Serotonin Receptor. *Anal. Chem.,* **81**, 3843 (2009).	
8	**S. Karthikeyan** and K. S. Kim, Structure, Stability, Thermodynamic Properties, and IR Spectra of the Protonated Water Decamer H+(H2O)10. *J. Phys. Chem. A*, **113**, 9237 (2009).	2.883
9	M. Guin, G. N. Patwari, **S. Karthikeyan** and K. S. Kim, A π-Stacked Phenylacetylene and 1,3,5-Triazine Hetero Dimer. A Combined Spectroscopic and Ab-initio investigation. *Phys. Chem. Chem. Phys.***11**, 11207 (2009).	3.829
10	S. Maity, G. N. Patwari, **S. Karthikeyan** and K. S. Kim, Binary Complexes of Tertiary Amine with Phenylacetylene. Dispersion win over Electrostatics. *Phys. Chem. Chem. Phys.***12**, 6150 (2010).	4.449
11	**S. Karthikeyan** and K. S. Kim, Structure, stabilities, thermodynamic properties and IR spectra of the acetylene clusters (C2H2)n=2-5. *J. Chem. Theory Comput.* **6**, 3190 (2010)	5.399
12	S. Maity, G. N. Patwari, **S. Karthikeyan** and K. S. Kim, A Combined Spectroscopic and Ab-initio Investigation of Phenylacetylene-Methylamine Complex. Observation of σ and π Type -Bonded Configurations and Fluorescence Quenching by Weak C–H•••N Hydrogen Bonding. *J. Phys. Chem. A*, **114**, 11347 (2010).	2.883
13	M. Guin, **S. Karthikeyan**, G. N. Patwari and K. S. Kim, Do N-Heterocyclic Aromatic Rings Prefer π-Stacking? *Phys. Chem. Chem. Phys.* **13**, 5514 (2011).	4.449
14	**S. Karthikeyan,** S. Robert, and P. Hobza, On the nature of stabilization in weak, medium and strong charge-transfer complexes: CCSD(T)/CBS and SAPT calculations. *J. Phys. Chem. A.* **115**, 9422 (2011). **(Most read article)**	2.883
15	A. Anthonysamy, Y. Lee, B. Karunagaran, S.-W. Rhee, **S. Karthikeyan** , K. S. Kim, and J. K. Kim, Molecular design and synthesis of Ruthenium(II) sensitizers for High Efficient Dye-sensitized Solar Cells. *J. Mater. Chem.* **21**, 12389 (2011).	6.626
16	M. Kolaski, A. Zakharenko, **S. Karthikeyan**, and K. S. Kim, Structures, energetic, and IR spectra of monohydrated inorganic acids: Ab initio and DFT study. *J. Chem. Theory Comput.* **7**, 3447 (2011).	5.399
17	Kwang S. Kim, **S. Karthikeyan**, and J. N. Singh, How different are aromatic π-interactions from aliphatic π-interactions and non-π stacking interactions. *J. Chem. Theory Comput.* **7**, 3471 (2011).	5.399
18	**S. Karthikeyan**, and S. Nagase, Origin of the stability of Imidazole-Imidazole, Benzene-Imidazole, and Benzene-Indole dimer: CCSD(T)/CBS and SAPT	2.883

	calculations. *J. Phys. Chem. A*, **116**, 1694 (2012). **(Most read article)**	
19	B. K. Mishra, **S. Karthikeyan**, and V. Ramanathan, Tuning CH-π interaction by different substitution in benzene-acetylene complex. *J. Chem. Theory Comput.* **8**, 1935 (2012).	5.399
20	S. Kang, **S. Karthikeyan**, and J. Y. Lee, Enhancement of the hydrogen storage capacity of Mg(AlH4)2 by excess electrons: A DFT study *Phys. Chem. Chem. Phys.* **15**,1216 (2013).	4.449
21	B. Kang, **S. Karthikeyan**, D. J. Jang, H. Kim, and J. Y. Lee, Concerted Asynchronous proton transfer in H-bonding relay model: An implication of green fluorescent protein, Bull. Korean Chem. Soc. **34(7)**, 1961(2013).	0.982
22	**S. Karthikeyan**, V. Ramanathan, and B. K. Mishra, Influence of the substituent on the CH-pi interaction: Benzene-Methane complex. *J. Phys. Chem. A*, **117**, 6687 (2013).	2.883
23	**S. Karthikeyan**, and J. Y. Lee, Zn-Porphyrin based dyes for dye-sensitized solar cells. *J. Phys. Chem. A,* **117**, 10973 (2013). **(Most read article)**	2.883
24	**S. Karthikeyan**, and J. Y. Lee, Tuning the C-X…π Interaction Benzene-Chloroacetylene complexes by Aromatic substitutions, *Chem. Phys*. Letts. , **602**, 16 (2014).	2.145
25	**S. Karthikeyan**, and J. Y. Lee, Benzotriazole-based based dyes containing a low band gap for dye-sensitized solar cells: A theoretical study, *Mol. Phys*., **112 (24),** 3120-3126 (2014).	1.837
26	K. L. V. Joseph, A. Anthonysamy, V. Ganapathy, **S. Karthikeyan**, S.-W. Rhee, K. S. Kim, and J. K. Kim, Cyanoacetic Acid Tethered Thiophene for Well-Matched LUMO level in Ru(II)-Terpyridine Dye Sensitized solar cells, *Dyes and pigment* **126,** 270-278 (2016).	4.055
27	J. Pitchaimani, A. Kundu, **S. Karthikeyan**, D. Moon, Madhu, P. Anthony, A Crab Claws Shaped Molecular Receptor for Selective Recognition of Picric Acid: Supramolecular Self-Assembly Mediated Aggregation Induced Emission and Color Change CrystEng*Comm.* **19**, 3557- 3561 (2017).	3.474
28	A. Karuppasamy, **S. Karthikeyan**, V. Pillai C. Ramalingan, Synthesis, spectral, structural prediction and computational studies of octylcarbazole ornamented 3-phenothiazinal, *Journal of Molecular Structure*,**1147**, 487-494(2017).	1.753
29	A. Kundu, **S. Karthikeyan**, D. Moon, P. Anthony, Self-reversible thermofluorochromism of D-A-D triphenylamine derivatives and effect of	3.474

	molecular conformation and packing. CrystEng*Comm.* **19**, 6979- 6985 (2017).	
30	P.S. Hariharan, P. Gayathri, A. Kundu, **S. Karthikeyan**, D. Moon, P. Anthony, Synthesis of tunable, red fluorescent aggregation enhanced emissive organic fluorophores: Stimuli responsive high contrast off-on fluorescence switching. CrystEng*Comm.* **20**, 643- 651 (2018).	3.474
31	A. Kundu, **S. Karthikeyan**, D. Moon, P. Anthony, Excited State Intramolecular Proton Transfer Induced Fluorescence in Triphenylamine Molecule: Role of Structural Conformation and Reversible Mechanofluorochromism, *Journal of Molecular Structure*, **1169**, 1-8 (2018).	1.753
32	S. Hariharan, P. Gayathri, A. Kundu, **S. Karthikeyan**, S. Yoshimitsu, D. Moon, P. Anthony, Drastic Modulation of Stimuli-Responsive Fluorescence by a Subtle Structural Change of Organic Fluorophore and Polymorphism Controlled Mechanofluorochromism, *Cryst. Growth Des.*,**18(7)**, 3971-3979 (2018).	4.055
33	A. Kundu, **S. Karthikeyan**, D. Moon, P. Anthony, Molecular Conformation – and Packing-Controlled Excited State Intramolecular Proton Transfer Induced Solid – State Fluorescence and Reversible Mechanofluorochromism, *Chemistry Select*, **3**, 1-7 (2018).	1.716
34	A. Kundu, **S. Karthikeyan**, D. Moon, P. Anthony, Unusual Fluorescent photoswitching of imidazole derivatives: Role of molecular conformation and twist angle controlled organic solid state fluorescence, *Phys. Chem. Chem. Phys.* **20**, 27385-27393 (2018).	3.902
35	A. Kundu, **S. Karthikeyan**, Y. Sagara, D. Moon, P. Anthony, Temperature-Controlled Locally Excited and Twisted Intramolecular Charge-Transfer State-Dependent Fluorescence Switching in Triphenylamine–Benzothiazole Derivatives, ACS Omega, **4(3)**, 5147-5154 (2019).	2.584
36	P. Gayathri, **S. Karthikeyan**, D. Moon, and P. Anthony, Halogen Atom and Position Dependent Strong Enhancement of Solid-State Fluorescence and Stimuli Responsive Reversible Fluorescence Switching, *Chemistry Select*, **4(13)**, 3884-3890 (2019).	1.716
37	M. J. Lee, N. K. Shee, J. I. Son, **S. Karthikeyan**, K. H. Jhee, J. Y. Lee, and H. J. Kim, Supramolecular complexation of homocysteine and cysteine with cucurbit[7]uril, *Journal Supramolecular chemistry*, **31(6)**, 369-376 (2019).	1.820
38	K. L. V. Joseph, N. T. Mary, R. Eswarmoorthi, **S. Karthikeyan**, and J. Kim, Output Current Enhancement of Hexylthiophene Functionalized D-π-Extended-A Triphenylamine in Dye Sensitized Solar Cells, *New J. Chem*, 43, 10834-10840(2019).	3.277

39	J. Pitchaimani, **S. Karthikeyan**, N. Lakshminarasimhan, S. Philip Anthony**,** D. Moon, V. Madhu, Reversible Thermochromism of Nickel(II) Complexes and Single-Crystal-to-Single-Crystal Transformation, ACS Omega, **4(9)**, 13756-13761 (2019).	2.584
40	P. Gayathri, **S. Karthikeyan**, M. Pannippara, A. Al-Sehemi, D. Moon, and P. Anthony, Aggregation Enhanced Emissive Mechanofluorochromic Carbazole-Halogen Positional Isomers: Tunable Fluorescence via Conformational Polymorphism and Crystallization Induced Fluorescence Switching, CrystEng*Comm.* **21**, 6604- 6612 (2019).	3.474
41	A. Kundu, **S. Karthikeyan**, D. Moon, and P. Anthony, Synthesis of Strongly Fluorescent Imidazole Derivatives: Structure Property Studies, Halochromism and Fluorescent Photoswitching, J. Fluoresc., **21**, 1-11 (2019).	1.913
42	P. Hariharan, C. Pen, **S. Karthikeyan**, A. Shinhara, and P. Anthony, Solvent vapour induced rare single-crystal-to-single-crystal transformation of stimuli-responsive fluorophore: Solid state fluorescence tuning, switching and role of molecular, *Dyes and pigment* **174,** 108067 (2020).	4.055
43	P. Gayathri, R. Sasikala, S. Karthikeyan, M. Pannipara, AG. Al-Sehemi, D. Moon and S. Philip Anthony, Pyridine Nitrogen Position Controlled Molecular Packing and Stimuli-responsive Solid-State Fluorescence Switching: Supramolecular Complexation Facilitated Turn-on Fluorescence, CrystEng*Comm.* **24**, 2642- 2649 (2022).	4.076
44	P. Gayathri, R. Sasikala, S. Karthikeyan, M. Pannipara, AG. Al-Sehemi, D. Moon and S. Philip Anthony, CF3 H-bonding locked aromatic stacking of picric acid with mechanofluorochromic fluorophores: highly selective reusable sensor and rewritable fluorescence platform, *Mol. Syst. Des. Eng.***,** **7**, 1277- 1286 (2022). **https://doi.org/10.1039/D2ME00075J**	4.935
45	P. Gayathri, R. Sasikala, K. Akshaya, S. Karthikeyan, M. Pannipara, A. G Al-Sehemi, D. Moon, S. Philip Anthony, ESIPT geometrical isomers with distinct mechanofluorochromism and intra/intermolecular H-bonding controlled tunable fluorescence, CrystEng*Comm.* **24(46)**, 8126-8133 (2022).	4.076

46	P. Gayathri, R. Sasikala, K. Akshaya, S. Karthikeyan, M. Pannipara, A. G Al-Sehemi, D. Moon, S. Philip Anthony, Hexagon and network structured organic geometrical isomers with distinct intramolecular H-bonding and stimuli-induced self-reversible fluorescence switching, CrystEng*Comm.* (2022).(Accepted).	4.076
47	P. Gayathri, S. Karthikeyan, M. Pannipara, AG. Al-Sehemi, D. Moon and S. Philip Anthony, Structural Insight of Anthracene Orientation by Halogen Substitution: Impact on Solid-State Fluorescence and Stimuli-Induced Fluorescence Switching, Crystal Growth & Design, **22(9)**, 5432- 5440 (2022). https://doi.org/10.1021/acs.cgd.2c00531	4.076
48	P.Gayathri, P. Nantheeswaran, M. Mariappan, S. Karthikeyan, M. Pannipara, A. G. Al-Sehemi, D. Moon, S. Philip Anthony, Methoxy substituent facilitated wide solvatofluorochromism, white light emission, polymorphism and stimuli-responsive fluorescence switching in donor-π-acceptor, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, **286**, 121989 (2023).	4.098

News:

1. **S. Karthikeyan**, and J. Y. Lee, *J. Phys. Chem. A.* **117**, 10973 (2013) paper was one of the 5 TOP most download article.
2. **S. Karthikeyan**, and S. Nagase, *J. Phys. Chem. A.* **116**, 1694 (2012) paper was one of the 5 TOP most download article.
3. **S. Karthikeyan,** S. Robert, and P. Hobza, *J. Phys. Chem. A.* **115**, 9422 (2011) paper was one of the 5 TOP most download article.

Invited Talk:

Department of Physics and Astronomy, **Uppsala Universitet**, **Sweden**, May 21-23, 2012.

a) Calculating intensities using effective Hamiltonian in terms of Coriolis-adapted normal modes
b) Strong Manifestation of Non-Covalent Interactions: From Clusters to Carbon Nano-Structures

Conference Presentations

1. **S. Karthikeyan**, and K. Mangala Sunder (International Symposium on Spectroscopy, Structure and Dynamics, (ISSSD), Dec 2002, IACS, Kolkatta, INDIA), Rotational-vibrational coupling in semi-rigid polyatomic molecules and molecular dipole moment.
2. **S. Karthikeyan** and K. Mangala Sunder (National Symposium in Chemistry, NSC, IIT Kanpur, Feb 2004, Kanpur) Calculation of rotational-vibrational intensities of polyatomic molecules using

new, effective dipole moment operators.

3. **S. Karthikeyan** and K. Mangala Sunder (National Symposium in Chemsitry, NSC, IACS Kolkatta, Feb 2005, Kolkatta) Calculation of rotational-vibrational intensities of ethylene using new, effective dipole moment operator.
4. **S. Karthikeyan** and K. Mangala Sunder (Discussion Meeting on Advanced Spectroscopy, *Indian Institute of Science*, Bangalore, Feb 2005, Bangalore) Calculations of rotational-vibrational intensities of ozone molecule using new, effective dipole moment operator in the presence of strong coriolis coupling.
5. **S. Karthikeyan** (Symposium/Workshop of Computational Science (SWOCS, Pohang University of Science and Technology (POSTECH), Nov 2009, South Korea), Structure, stabilities, thermodynamics properties and IR spectra of Acetylene (C2H2)n=2-5 clusters
6. **S. Karthikeyan**, P. Hobza (Symposium/Workshop of Computational Science (SWOCS, Pohang University of Science and Technology (POSTECH), Nov 2010, South Korea).
7. **S. Karthikeyan**, J. Y. Lee, Korean Chemical Social (KCS) Meeting, Goyang, April 17-20, 2013, South Korea.
8. **S. Karthikeyan**, International Conference on Advanced Material Science and Technology (ICAMST), Banari Amman Institute of Technology, Tamil Nadu, India. August 17-19, 2017.
9. **S. Karthikeyan**, 4th International Conference on Chemical and Environmental Research (ICCER- 2018), Jamal Mohamed College, Trichy – 20, Tamil Nadu, India. December 19, 2018.

Workshop:

1. **S. Karthikeyan**, "Advanced Teaching Methodologies", Centre for Learning Technology, 10 March, 2017.
2. **S. Karthikeyan**, "Recent Research Issues in Bio-Informatics and Bio-sensor, Department of Computer Applications & Centre for Learning Technology, 17 March, 2017.
3. **S. Karthikeyan**, "IT skills enrichment for young chemists" Department of chemistry & Computer science and engineering, Kalasalingam University, 24 March, 2017.
4. **S. Karthikeyan**, "Art of Counselling and Mentoring", Centre for Learning Technology, 20 June, 2017.
5. **S. Karthikeyan**, "Training Methodology & Creative Thinking", Centre for Learning Technology, 19-21 December, 2017.

Membership: Life member-Association of Environmental Analytical Chemistry of India (AEACI), Bhabha Atomic Research Centre, Mumbai, India.

Details of Book Publication -

Chairman / Member Board of Studies in University / Autonomous Colleges :-

Computer Skills

1	Operating Systems	: Unix, Linux, Windows
2	Programming languages	: Fortran 77, Matlab
3	Scientific packages	: Gaussian 09, Molpro 2009.1, Turbomole 6.0, SAPT, GAMESS, Amber, Cerius 2, Chem Draw 9.0, POSMOL, MOLMOL, Orgin 8, ChemCraft. Mercury Chemissian.
4	Documentation	: Latex, MS office

References

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Date: Signature

(Dr. S.Karthikeyanann)