## **CURRICULUM VITAE**

Dr. V. TAMILMANI **Assistant Professor Department of Chemistry** 

UCE - BIT Campus, Tiruchirappalli 620 024

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### > Research Area:

- Theoretical and Computational Chemistry
- Quantum Chemistry of Chemical Reactions and Complexes Transition State Modeling Ionic Cycloadditions- Studying Solvent effect in Chemical Reactions – Density Functional Theory- Organic Solar Cells

# > Educational Qualifications:

| Qualification          | College/University                                 | Year of completion | Percentage          | Class |
|------------------------|--|--------------------|---------------------|-------|
| Ph.D. (specialization) | Bharathidasan<br>University                        | 2007               | Highly<br>Commended |       |
| M.Phil.                | Bharathidasan<br>University                        | 2001               | 72                  | I     |
| PG (specialization)    | Govt College for Men<br>(Autonomous)<br>Kumbakonam | 1999               | 64.7                | I     |
| UG (specialization)    | Govt College for<br>Women, Kumbakonam              | 1997               | 64.3                | I     |
| Others                 |  |                    |                     |       |

**Experience:** (chronological order)

| Name of Company /<br>Institutions | Designation of Post | From | То | Experience in<br>Year |
|-----------------------------------|---------------------|------|----|-----------------------|
|                                   |                     |      |    |                       |
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|                                   |                     |      |    |                       |

## > Awards / Honours Received:

- 1. Senior Research Fellow, CSIR
- 2. Swiss Federal Commission Scholarship for Foreign Students
- 3. SCS Best Poster ward

# > Additional / Academic Responsibilities at University:

- 1. YRC Programme Officer from 2009 July 2015.
- 2. Member in Anti Ragging committe in the year 2012-2013.

# > Fellowships and Grants received:

- **1. Senior Research Fellow in CSIR Project**, School of Chemistry, Bharathidasan University, Tiruchirappalli 620 024, Tamil Nadu, India. (*Dec 2002-July 2003*)
- **2. COST-STSM**, Laboratoire de Chimie Quantique , University of Louis Pasteur, Strasbourg, France. (*September 2004 -October 2004*) Funded by *European Science Foundation*

# > Research Guidance (M.S/Ph.D.) (Completed):

| S1.   | Name of the                     | Title of the thesis   | Year of      | Date of    |
|-------|---------------------------------|---|--------------|------------|
| No    | scholar                         |   | registration | viva voce  |
| 1. 2. | D. Gajalakshmi<br>A. Adilakshmi | DFT/ TDDFT Design and<br>Evaluation of Heterocyclic<br>Oligomers for Optoelectronic and<br>Anti- Corrosion Applications | 2011         | 08.05.2017 |
|       |                                 | Modelling [4+2] Cycloaddition<br>Reactions of 2-<br>Bromocycloalkenones   | 2011         | 12.02.2020 |

## > Publications:

a. Books / book chapters:

#### b. International Journals:

- 1. Hydrogen bond stabilization in Diels-Alder transition states: The cycloaddition of hydroxy-ortho-quinodimethane with fumaric acid and dimethyl fumarate, **V. Tamilmani**, C. A. Daul, J. Lage Robles, C. G. Bochet and P. Venuvanalingam, *Chem. Phy. Lett* (2005) 406(4-6), 355. [Impact Factor 2.21]
- 2. An ab initio and DFT study on the hydrolysis of carbonyl dichloride S. Mahesh, G. Rajaraman, J. Prabha, V. Tamilmani and P. Venuvanalingam. Journal of Molecular Structure: THEOCHEM, (2005) 730, 155. [Impact Factor 1.045]
- 3. Electrostatic Control on endo/exo Selectivity in Ionic Cycloadditions, **V.Tamilmani**, C.A.Daul and P.Venuvanalaingam, *Chem. Phy. Lett*, **(2005)** 416, 354. [Impact Factor 2.21]
- 4. Possible Ring Structures of Armchair Single Walled Carbon Nanotubes. **V.Tamilmani**, C.A.Daul and T.Jenny, *Chimia*(**2006**) 60, 228. [Impact Factor 0.626]
- 5. A DFT based ligand field study of EPR spectra of Co(II) and Cu(II) porphyrins. Mihail Atanasov a,c, Claude A. Daul, Marie-Madeleine Rohmer, **Tamilmani** Venkatachalam *Chem. Phy. Lett*, (2006) 427, 449. [Impact Factor 2.33]
- 6. A DFT/ TDDFT Mission to Probe Push-Pull Vinyl Coupled Thiophene Oligomers for Optoelectronic Applications, Duraikannu Gajalakshmi, Rajadurai Vijay Solomon, Venkatachalam **Tamilmani**, Mariasusai Boobalan, Ponnambalam Venuvanalingam. RSC Adv ( **2015**) 5, 50353. [Impact Factor 3.289]
- 7. Unraveling the Role of Π Conjugation in Thiophene Oligomers for Optoelectronic Properties by DFT/TDDFT Approach, D. Gajalakshmi and **V. Tamilmani**, *Brazilian Archives of Biology and Technology*, (**2016**) 59. [Impact Factor 0.744].
- 8. Theoretical Investigation of Steric Effect Influence on Reactivity of Substituted Butadienes with Bromocyclobutenone, A. Adilakshmi, M. Deepan Kumar, M. Jaccob, V. Tamilmani, J. Chem. Inf. Model. (2019) 59, 5, 2231-2241 [Impact Factor 3.966].
- Are vinyl coupled furan derivatives better than vinyl coupled thiophene derivatives for optoelectronic applications? -Answers from DFT/TDDFT calculations, D. Gajalakshmi , M. Boobalan, R. Vijay Solomon, V. Tamilmani, Com. Mat. Sci (2019) 162, 60–68 [Impact Factor 2.644].

#### c. National Journals:

- Nnbnn Stereoselectivity in Cationic Cycloadditions.
   V.Tamilmani, D.Senthilnathan and P.Venuvanalingam, *J. Chem. Sci*(2008) 120, 1.
   [Impact Factor 0.745]
- 2. Biocatalysis of azidolysis of epoxides:Computational evidences on the role of Halohydrin dehalogenase (HheC). Senthilnathan, D, **Tamilmani**, V and Venuvanalingam, P. *J. Chem. Sci.*, (2011)123, 279. [Impact Factor 1.177]
- 3. Blending Ratio of Low Sulphur Diesel: A Key to Lower Emissions, A. Adilakshmi, V. Venkatesan and V. Tamilmani, Journal Industrail Pollution Control (2014) 30, 139.

# > List of Seminar / Short Term Course /FDP/ Workshop organized:

- TEQIP II sponsored two day Seminar on Challenges & Opportunities in Chemical and Environmental Research (Chemera 2016) on11<sup>th</sup>& 12<sup>th</sup> August 2016.
- Organized One day Workshop on *Sustainability Agriculture and the Impacts on Environment* on 3<sup>rd</sup> October 2019

## > List of Seminar / Short Term Course /FDP/ Workshop attended:

- ➤ Participated in JNCASR Frontier Lecture Series conference held in Bharathidasan Tiruchirappalli, India during Dec 16-18, **1998**. (2days)
- ➤ Participated in the workshop on *Latex* held in St- Joseph College, Tiruchirappalli, India on 27<sup>th</sup> Jan, 2003.
- ➤ Participated in State Level seminar on Challenges and applications in Bioinformatics held in Bharathidasan University, Tiruchirappalli, India during 31<sup>st</sup> March 1<sup>st</sup> April, 2003. (2days)
- ➤ Participated in the Workshop on *Soft Skills* held in PeriyarManiammai University, Thanjavur on 25<sup>th</sup> July, 2009.
- ➤ Participated in the seminar on "*Recent Developments in Chemistry*" held on 29<sup>th</sup> August, **2011** at Bharathidasan University, Tiruchirappalli.

- Attended in UGC sponsored **Orientation Programme** Conducted by Academic Staff College, Bharathidasan University University, Tiruchirappalli. during **1.2.2013 to 28.02.2013.** (28 Days)
- ➤ Attended TEQIP II sponsored one week Faculty Development programme on "Current Developments in Life Sciences An Interdisciplinary Approach CCDLS-2013" Organized by Department of Pharmaceutical Technology, BIT campus Anna University Tiruchirappalli during 19<sup>th</sup> 25<sup>th</sup> August **2013.** (**7 Days**)
- ➤ Participated two days lecture workshop on "Recent Advances In Materials Chemistry" (RAMC'14) held at Department of Chemistry, Bharathidasan Institute of Technology, Anna University, Tiruchirappalliduring March 7 & 8, 2014. (2 days)
- Attended TEQIP II sponsored two weeks Faculty Development Programme on "Nano Technology Applications in Engineering and Technology (NAET'15)" Organized by Department of Petrochemical Technology, BIT campus, Anna University, Tiruchirappalliduring 6<sup>th</sup> to 19<sup>th</sup> May **2015**. (15 days)
- Attended TEQIP II sponsored course on "Faculty Development Programme" on 1<sup>st</sup> March **2016**, Organized by Bharathidasan Institute of Technology, Anna University, Tiruchirappalli-620 024 in association with Confederation of Indian Industry(CII) (1 Day)
- Attended TEQIP II sponsored two day lecture workshop on "Chemistry for Sustainable Green Environment (CHES GREEN'16)" Organized by Department of Chemistry, BIT campus, Anna University, Tiruchirappalliduring 11<sup>th</sup> to 12<sup>th</sup> March **2016**, (2days)
- ➤ Attended TEQIP II sponsored two weeks *Faculty Development Programme*om "Multi-disciplinary approaches in Chemical Sciences (MACS- 2016) organized by Department of Chemistry, BIT campus, Anna University, Tiruchirappalli during 18<sup>th</sup> to 31<sup>th</sup>July**2016**, (15days)
- Attended 3<sup>rd</sup> National Seminar on "Advanced Oxidation Processes (AOP 2017)" Organized by Department of Chemistry, BIT campus, Anna University, Tiruchirappalli. during 17<sup>th</sup> -19<sup>th</sup> December 2017 (2 days)
- ➤ Attended in UGC sponsored **Refresher Course in Nano Sciences con**ducted by Academic Staff College, Bharathidasan University University, Tiruchirappalli. during 20.12.2018 to 06.01.2018. (21 Days)

- "DFT/TDDFT Design and Evaluation of Heterocyclic Oligomers for Optoelectronic and Anti-Corrosion Application"
- ▶ has been accepted for the Oral presentation in the International Conference on Recent Trends in Materials and Magnetism (RTMM-22) on 15<sup>th</sup> December 2022 at Loyola College Chennai.
- National / International Conferences organized / Participated:
- ➤ **Professional recognitions:** (details like chairperson/member of a committee, reviewer, editor ...etc)
- (A) Chairperson for conferences / Seminar / Technical symposia:
- (B) Guest lectures delivered:
- (C) Invited Speaker at KKC engineering college, one day seminar "Come Chem World", Jayankondam on 09.03.2013.
- (D) As a resource person for a FDP on Engineering Chemistry II 16.12.2014 UCE- Thirukuvalai Campus.
- (E) Delivered Invited Lecture on 28<sup>th</sup> Feb, 2020 in Winter School on Computational Modelling held at Department of Physics, Holy Cross College (Autonomous), Tiruchirappalli, during 27<sup>th</sup>-29<sup>th</sup> February 2020.
- (F) Delivered Invited Lecture on 25<sup>th</sup> June, 2022 in Department Association on Evaluation of Heterocyclic Oligomers for Optoelectronic and Anti-Corrosion held at Department of Chemistry, Seetha Lakshmi Ramasamy College (Autonomous), Tiruchirappalli.

## **Visits Abroad:**

- Department of Chemistry, University of Fribourg, Switzerland during (*July 2003- Oct 2005*) through Swiss Federal Commission Scholarship.
- Laboratoire de Chimie Quantique, University of Louis Pasteur, Strasbourg, **France**. (September 2004 October 2004) Funded by European Science Foundation (COST-STSM)

| • Department of Chemistry, Sookmyung Women's University, Seoul, <b>Korea</b> on <i>October 200</i>                          | 7    |
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| <b>DECLARATION:</b> I certify that the information furnished above is correct and true to the best of my knowle and belief. | edge |
| Signature of the staff mem  | ıber |
| Head of the Department Dean   |      |
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