

# Dr. Prabha Vadivelu

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**Personal Profile:** Date of Birth: **22-05-1979** Sex: **Female** Marital status: **Married** Nationality: **Indian**.

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## EXPERTISE IN

- Computational modelling of organic/inorganic/bioinorganic complexes and reaction mechanisms.
- Handling open shell complexes (non-heme iron, Ruthenium, Nickel), spin state ordering, single/multiple spin state reactivity.
- DFT, ADF, semiempirical, ab-initio and Molecular Mechanics methods.
- Teaching Physical chemistry for undergraduate and postgraduate students.
- Attracting funding from external agencies.
- Publishing papers in peer-reviewed international journals.

## EDUCATION

- **Ph.D., Chemistry Department, Heriot-Watt University**, Edinburgh, UK (Oct 2003 – May 2007).  
Supervisor: Dr. Stuart. A. Macgregor.  
Thesis title: *Theoretical studies on the reaction of low-valent transition metal alkoxides and amides*.
- **M.Sc. Chemistry, Bharathidasan University**, Trichirapalli, India (June 2001 - May 2003).  
Supervisor: Professor P. Venuvanalingam.  
Dissertation title: *Effect of Lewis Acid Catalyst in the Cycloaddition of Methyl Vinyl Ketone and Ketene*.
- **B.Sc. Chemistry, Bharathidasan University**, Trichirapalli, India (July 1998 - May 2001).

## HONORS AND AWARDS

- Distinction and obtained **Gold medal** in Bachelor's degree (2001).
- Awarded **Summer Fellowship** from the Indian Academy of Sciences, Bangalore (2002).
- **University second rank** in Master's Degree (2003).
- Recipient of **James-Watt Scholarship** from Heriot-Watt University (2003-2006).
- Selected as a young scientist to attend the **Nobel Laureates meetings**, Lindau, Germany. (June 28- July 3, 2009).

## EXTERNALLY FUNDED PROJECT

1. **Project Title:** Utilization and activation of CO<sub>2</sub> via transition metal-mediated insertion reactions: A Computational study (**Completed**)
  - **Funding Agency:** DST-SERB, India
  - **Budget:** Rs. 31,20,000/-
  - **Period of operation:** Dec-2013 to Nov-2016
2. **Project Title:** Pd-catalysed selective aromatic halogenation reactions - A DFT study (**Completed**)
  - **Funding Agency:** UGC, India.
  - **Budget:** Rs. 10,00,000/-
  - **Period of operation:** Feb-2019 to Jan-2021
3. **Project Title:** Utilization and Transformation of CO<sub>2</sub>: A DFT study on Pd- and Ni-catalysed carboxylation of organic halides with CO<sub>2</sub>. (**Completed**)
  - **Funding Agency:** DST-SERB, India.
  - **Budget:** Rs. 28,54,000/-
  - **Period of operation:** March-2019 to Feb-2022

## TEACHING AND RESEARCH EXPERIENCE

**Nov 2017 - At present: Assistant Professor (regular)**, Department of Chemistry, Central University of Tamilnadu, Thiruvavur, Tamilnadu.

- Teaching physical chemistry to i.MSc and MSc students and conducting laboratory sessions.
- Mentoring MSc and PG diploma project students.
- Attracting external research funding.
- Publishing research articles in peer-reviewed international journals.

**Dec 2013 – Nov 2016: DST- Fast Track Young Scientist**, CSIR – National Institute for Interdisciplinary Science and Technology (NIIST), Trivandrum, Kerala, India.

*Software used* : G09 and chemcraft.

- Designed CO<sub>2</sub> activation and fixation catalyst based on Ru and Ir metal complexes.
- Predicted CO<sub>2</sub> insertion mechanism.
- Investigation of metal-free organic catalysts and their ability for cyclic carbonate formation.
- Published nearly 6 research articles in this project and 3 of them with the corresponding authorship.

**Jan 2012 - May 2012: Assistant Professor (Senior)** at the VIT University, Vellore, Tamil Nadu, India.

*Responsibilities*: (i) Giving Lectures to Undergraduate and Postgraduate engineering and science students, (ii) Writing research grants.

**Nov 2010 - May 2011: Guest Scientist** at the University of Manchester, Manchester, United Kingdom.

*Software used*: Orca, G03 and Jaguar.

- Modelled the antiferromagnetic wheel complex of [R<sub>2</sub>NH<sub>2</sub>][Cr<sub>7</sub>CuF<sub>8</sub>((O<sub>2</sub>Me)<sub>16</sub>]
- Investigated the spin coupling pattern and also identified the Jahn-Teller distortion axis.

**June 2007 - Nov 2009: Post doctoral fellow** at the University of Heidelberg, Heidelberg, Germany.

*Software used*: G03, Jaguar 6.5. ADF, Macromodel and Momec.

- Modelled several biologically active and bio-mimicking model complexes viz. [(L)Fe<sup>IV</sup>=O(OH)]<sup>+</sup>, [(L)Fe<sup>V</sup>=O(OH)]<sup>2+</sup>, [(L)Ru<sup>IV</sup>=O(OH)]<sup>+</sup> and [(L)Ru<sup>IV</sup>=O]<sup>2+</sup> where L = tetradentate and pentadentate bispidine ligand.
- Investigated the Non-heme iron and ruthenium-mediated alkane hydroxylation and alkene epoxidation reaction mechanisms.
- Predicted the active catalyst (Fe-oxo species) with the preferred oxidation and spin-state configuration.
- Found out the two-spin state reactivity and spin-cross over mechanism.
- Carried out the conformation analysis (using Macromodel and Momec) and DFT calculations of the macrocyclic patellamides (pseudo octapeptides) complexes for studying the Cu(II) coordination mode, the conformational flexibility and their ability towards CO<sub>2</sub> fixation.

## PUBLICATIONS

1. Stuart A. Macgregor and **Prabha Vadivelu**, “Computational studies on the relative stabilities of *trans*-Ir(PPh<sub>3</sub>)<sub>2</sub>(CO)OR and *trans*-Ir(PPh<sub>3</sub>)<sub>2</sub>(CO)CH<sub>2</sub>R towards β-Hydrogen elimination” *Organometallics*, 2007, 26(15), 3651-3659. IF – 4.126
2. Simon K. Brayshaw, Thomas M. Douglas, Romaeo Dallanegra, Gemma L. Moxham, Gabriele Kociok-Köhn, and Andrew S. Weller, Stuart A. Macgregor, **Prabha Vadivelu** and Tebikie Wondimagegn “Intramolecular Alkane Dehydrogenation in Cationic Rhodium Complexes of Tris-Cyclopentylphosphine” *Chem. Eur. J.*, 2008, 14, 1004-1022. IF – 5.731
3. Peter Comba, Martin Maurer and **Prabha Vadivelu**, “Oxidation of cyclohexane by a high-valent iron bispidine complex a combined experimental and computational mechanistic study” *J. Phys. Chem. A*, 2008, 112(50), 13028-13036. IF – 2.693

4. Jordi Benet-Buchholz, Peter Comba, Antoni Llobet, Stephan Roeser, **Prabha Vadivelu**, Hubert Wadepohl and Sebastian Wiesner, "Iron versus Ruthenium – A Comparison of the Stereoselectivity in the Catalytic Olefin Epoxidation" *Dalton Trans*, 2009, 5910-5923. IF – 4.197
5. Peter Comba, Martin Maurer and **Prabha Vadivelu**, "Oxidation of Cyclohexane by High-Valent Iron Bispidine Complexes: Tetradentate versus Pentadentate Ligands" *Inorg. Chem*, 2009, 48(21), 10389-10396. IF – 4.762
6. Jordi Benet-Buchholz, Peter Comba, Antoni Llobet, Stephan Roeser, **Prabha Vadivelu** and Sebastian Wiesner, "The RuIV=O-catalyzed sulfoxidation: a gated mechanism where O to S linkage isomerization switches between different efficiencies" *Dalton Trans*, 2010, 39, 3315-3320. IF – 4.197
7. Michael L Baker, Stergios Piligkos, Alberto Bianchi, Stefano Carretta, David Collison, Joseph J. W McDouall, Eric J. L. McInnes, Hannu Mutka, Grigore A. Timco, Floriana Tuna, **Prabha Vadivelu**, Høgni Weihe, Hans U. Güdel, and Richard E. P. Winpenny, "Modification of the magnetic properties of a heterometallic wheel by inclusion of a Jahn-Teller distorted Cu(II) ion" *Dalton Trans*, 2011, 40(34), 8533-8539. IF – 4.197
8. Madhavan Jaccob, Peter Comba, Martin Maurer, **Prabha Vadivelu**, and Ponnambalam Venuvanalingam, "A combined experimental and computational study on the sulfoxidation by high-valent iron bispidine complexes" *Dalton Trans*, 2011, 40(42), 11276-11281. IF – 4.197
9. Peter Comba, Lawrence R. Gahan, Gebhard Haberhauer, Graeme R. Hanson Christopher J. Noble, Björn Seibold, and **Prabha Vadivelu**, "Cu<sup>II</sup> coordination chemistry of patellamide derivatives. Possible biological functions of cyclic pseudo-peptides" *Chem. Eur. J*, 2012, 18, 2578-2590. IF – 5.731
10. Muniyandi Sankaralingam, Prabha Vadivelu, Eringathodi Suresh, Mallayan Palaniandavar, "Mixed ligand nickel(II) complexes as catalysts for alkane hydroxylation using *m*-chloroperbenzoic acid as oxidant" *Inorganica Chimica Acta*, 2013, 407, 98-107. IF – 2.046
11. Muniyandi Sankaralingam, Mani Balamurugan, Mallayan Palaniandavar\*, **Prabha Vadivelu\***, Cherumuttathu H. Suresh, "Nickel(II) Complexes of Tripodal 5N Ligands as Catalysts for Alkane Hydroxylation using *m*-CPBA as Oxidant: A Combined Experimental and Computational Study", *Chem. Eur. J*, 2014, 20, 11346-11361. IF – 5.731
12. Mani Balamurugan, **Prabha Vadivelu** and Mallayan Palaniandavar, "Iron(III) Complexes of Tripodal Tetradentate 4N Ligands as Functional Models for Catechol Dioxygenases: Electronic Vs Steric Effect on Extradiol Cleavage" *Dalton Trans*, 2014, 43, 14653-14668. IF – 4.197
13. **Prabha Vadivelu\*** and Cherumuttathu H. Suresh "Metal- and ligand-assisted CO<sub>2</sub> insertion into Ru-C, Ru-N and Ru-O bonds of Ru(II) phosphine complexes: A DFT Study" *Inorg. Chem*, 2015, 54, 502-512. IF – 4.762
14. **Prabha Vadivelu\*** and Cherumuttathu H. Suresh "Computational prediction of cyclometalated Ir<sup>III</sup>, Rh<sup>III</sup> and Co<sup>III</sup> amido complexes to capture up to three CO<sub>2</sub> molecules" *Dalton Trans*, 2015, 44, 16847-16853. IF – 4.197
15. Muniyandi Sankaralingam, **Prabha Vadivelu**, Mallayan Palaniandavar, "Novel nickel(II) complexes of sterically modified linear N<sub>4</sub> ligands: Effects of donor atom type, steric hindrance, diamine backbone and solvent on nickel(II) spin state and alkane hydroxylation with *m*-CPBA as oxidant" *Dalton Trans*, 2017, 46, 7181-7193. IF – 4.197
16. Gejo George, Suja Bhargavan Sisupal, Teenu Tomy, Alaganadam Kumaran, **Prabha Vadivelu**, Vemparthan Suvekbala, Swaminathan Sivaram and Lakshminarayanan Ragupathy, "Facile, environmentally benign and scalable approach to produce pristine few layers graphene suitable for preparing biocompatible polymer nanocomposites" *Scientific Reports*, 2018, 8, 11228. IF – 4.122
17. Panneerselvam Devibala, Ramachandran Dheepika, Prabha Vadivelu, and Samuthira Nagarajan, "Synthesis of Aroylbenzoate-Based Push-Pull Molecules for OFET Applications" *ChemistrySelect*, 2019, 4, 2339-2346. IF – 1.505. IF – 2.307
18. K. Ganesan, I. Kaliyaperumal, **P. Vadivelu\*** "A Density Functional Theory Study on Comparing the Reactivity of [Mn(13-TMC)(OOH)]<sup>2+</sup> and [Mn(13-TMC)(O<sub>2</sub>)]<sup>+</sup> for the Sulfoxidation of Thioanisole" *Inorg. Chem*, 2021, 60, 13615-13625. IF – 5.436
19. S. Krishnan, M. G. Maya, A. Das, S. Bhargavan, K. Ganesan, S. Sivaram, **P. Vadivelu\*** & L. Ragupathy\*, In-situ interfacial compatibilization via edge-sulfurated few-layer graphene during the formation of crosslinked graphene-rubber nanocomposites, *Scientific Reports*, 2022, 12, 4013. IF – 4.997

20. **P. Vadivelu\*** and K. Ganesan, “Density Functional Theory Study on [Ni<sup>0</sup>(1,10-Phenanthroline)]-Catalyzed Reductive Carboxylation of Alkyl and Aryl Halides with CO<sub>2</sub>: Effect of the Lewis Acid and β-H Elimination Side Reaction in the Crucial CO<sub>2</sub> Insertion Step” *Inorg. Chem.*, 2022, 61, 48, 19463-19474. IF – 5.436
21. Madavi S. Prasad, Sankar Bharani, Murugesan Sivaprakash, **Prabha Vadivelu**, Durairajan Siva Sundara Kumar and L. Raju Chowhan, , “*N*-2,2,2-Trifluoroethylisatin ketimine as a 1,2-dipolarophile for [3 + 2]-addition to access optically pure spirothiazolidine oxindoles” *Org. Biomol. Chem.* 2023, 21, 4972-4976. IF - 3.2
22. Thasnim P Mohammed, Akhila George, Madhuri Priya Sivaramakrishnan, **Prabha Vadivelu**, Sridhar Balasubramanian, Muniyandi Sankaralingam, “ Deciphering the effect of amine versus imine ligands of copper (II) complexes in 2-aminophenol oxidation” *J. Inorg. Biochem.* 2023, 247, 112309. IF-4.336

### SELECTED INVITED TALKS

- Presentation on “Exploring the mechanistic insights of Ru(II)-Mediated CO<sub>2</sub> Insertion Reactions and Ni(II)-Catalysed Alkane Hydroxylation – A DFT study” at MCBR4 meeting, Germany, Heidelberg, Feb 23-27, 2015.
- Presentation on “DFT study to explore mechanistic insights of transition metal-mediated C-H activation” at CUTN, Transition-2019, 22-23, Feb 2019.
- Presentation on “Computational Approaches for Experimental Chemists-2022” at VIT-Chennai, 17-18, March 2022.
- Presentation on “Photonics to Quantum Mechanics: Disappearing boundaries in research” at Government College Kariavattam, Trivandrum, Kerala, 12, Feb 2022.
- Presentation on “Role of DFT study in revealing the mechanistic insights of Ni- and Mn-based bio-mimetic complexes” at Loyola College, Chennai, 15-16 Dec-2022.
- Presentation on “Computational materials and molecular design” at CUTN in STUTI-21, 23 June-2023.

### FDP/OC/WORSHOPS ATTENDED

- Faculty development program on Carbon Capture & Storage, 21-25 Feb, 2022, CUTN
- Workshop on Techno-Pedagogical Tools & Techniques, 5-9 July, 2021, CUTN
- Refresher course held from 20<sup>th</sup> July-2<sup>nd</sup> August, 2021, Mizoram University.
- Orientation course held from 28<sup>th</sup> July – 17<sup>th</sup> August, 2020, Mizoram University.