

## Dr. ROJISHA V. C

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### ACADEMIC PROFILE:

| INSTITUTE  | UNIVERSITY/ BOARD                        | YEAR OF PASSING    |
|--|--|--------------------|
| <b>Ph.D.</b> ( <i>Theoretical Studies on the Structure, Bonding and Reactivity of Singlet Tetrylenes.</i><br><i>Supervisor: Dr. P. Parameswaran, NIT Calicut</i> ) |  |                    |
| National Institute of Technology Calicut   | National Institute of Technology Calicut | <b>August 2016</b> |
| <b>M. Sc Chemistry</b>   |  |                    |
| Malabar Christian College, Calicut   | University of Calicut                    | 2009               |
| <b>B. Sc Chemistry</b>   |  |                    |
| Providence Women's College, Calicut  | University of Calicut                    | 2007               |
| <b>Higher Secondary School</b>   |  |                    |
| Govt. Higher Secondary School East Hill  | Board of Higher Secondary Education      | 2004               |
| <b>Secondary School</b>  |  |                    |
| K.M.O. Higher Secondary School Koduvally   | State Board of Secondary Education       | 2002               |

### PROFESSIONAL RECOGNITION, AWARDS, FELLOWSHIPS RECEIVED:

- Qualified GATE, 2010 (561<sup>th</sup> All India Rank; 93.04 percentile).
- Qualified National Eligibility Test (NET) for Lectureship conducted by CSIR-UGC, December 2010.
- Awarded National Postdoctoral Fellowship (NPDF) by SERB, India – 2016

### DETAILS OF RESEARCH:

- **Research Area:** Computational Chemistry
- **Research Interests:**
  - Computational studies on coordination chemistry of main group elements, transition, and organometallic compounds.

- Quantum mechanical designing of ligands and catalysts.
- Theoretical investigations on organic and organometallic reactions.
- **Thesis Title:** Theoretical Studies on the Structure, Bonding and Reactivity of Singlet Tetrylenes. Supervisor: Dr. P. Parameswaran, NIT Calicut
- **Research Experience:**
  - Post-Doctoral Research at IIT Hyderabad (From October 2016- November 2017) under the guidance of Dr. Deva Priyakumar.
  - Research Scholar in the Department of Chemistry at National Institute of Technology Calicut (From 2010 December onwards) under the guidance of Dr. P. Parameswaran.
  - Project Fellow at National Chemical Laboratory, Pune (March 2009-May 2009) under the guidance of Dr. Kumar Vanka.

## FUNDED PROJECTS

Title of the project: Structures, Stabilities and Catalytic Activities of Surface Anchored Metal Nanoparticles: A Detailed Quantum Mechanical and Molecular Dynamics Study  
Funded by SERB India (PDF/2016/003480)

## LIST OF PUBLICATIONS:

1. "Electronic Structure of Six-Membered N-Heterocyclic Carbenes and Its Heavier Analogues: Reactivity of the Lone Pair versus the Exocyclic Double Bond"; **Rojisha, V. C.** De, S, Parameswaran, P. *Inorg. Chem.* **2012**, 51, 8265-8274.
2. "Singlet 2-Adamantylidene –An Ambiphilic Foiled Carbene Stabilized by Hyperconjugation"; **Rojisha, V. C.** Nijesh, K. De, S. Parameswaran, P. *Chem. Commun.*, **2013**, 49, 8465-8467.
3. "Intermolecular Interactions in Fluorinated Tetraarylporphyrins: An Experimental and Theoretical Study"; Soman, R. Sujatha, S. De, S. **Rojisha, V. C.**, Parameswaran, P. Varghese, B. Arunkumar, C. *Eur. J. Inorg. Chem.*, **2014**, 2653–2662.
4. "2-Adamantylidene and its Heavier Analogues: Hyperconjugation versus Lone Pair Stability and Electrophilicity versus Nucleophilicity" Nijesh, K.; **Rojisha, V. C.**; De, S.; Parameswaran, P. *Dalton Trans.* **2015**, 44, 4693-4706.
5. "Neutral cyclic alkyl amino carbenes stabilize rare chromium(I) centres " Roesky H. W.; Samuel P. P.; Neufeld R.; Mondal K. C.; Irme H. R.; Stalke D.; Demeshko S.; Meyer F.;

- Rojisha V. C.**; De S.; Parameswaran P.; Stückl A. C.; Kaim W.; Dalal N.; Christian J. H.; Bindra J. K.; **Chem. Sci.**, **2015**, 6, 3148-3153.
6. "Comparing Nucleophilicity of Heavier Heteroleptic Amidinato-Amido Tetrellylenes: An Experimental and Theoretical Study" Parvin, N.; Pal, S.; **Rojisha, V. C.**, De, .; Parameswaran, P.; Khan, S. **ChemistrySelect** **2016**, 1, 1991-1995.
  7. "Transition between [R]- and [S]-stereoisomers without bond breaking" Shampa Raghunathan, Komal Yadav, **V. C. Rojisha**, Tanashree Jaganade, V. Prathyusha, Swetha Bikkina, Upakarasamy Lourderaj, U. Deva Priyakumar **Phys. Chem. Chem. Phys.**, **2020**,22, 14983-14991.
  8. "Nature of CN bond in N-heterocyclic carbene" **Rojisha V. C.**, Purushothaman I., De S.; Parameswaran P, **Chem. Phys. letters**, **2021**, 765, 138312.

#### **POSTER PRESENTATIONS IN THE INTERNATIONAL CONFERENCES:**

1. Presented a poster on "Electronic structure and reactivities of N-heterocyclic six membered carbenes and its higher analogues" [ATOMS – 2011, 2<sup>nd</sup> - 5<sup>th</sup> Nov 2011 at IICT Hyderabad].
2. Presented a poster on "Electronic structure of six-membered N-heterocyclic carbenes and its heavier analogues: reactivity of lone-pair versus exocyclic double bond" [MCBR3 – 2013, 26<sup>th</sup> Feb – 1<sup>st</sup> Mar 2013 at NIPER & IISER Mohali].
3. Presented a poster on "2-Adamantylidene and its heavier analogues: hyperconjugation versus lone pair stability and electrophilicity versus nucleophilicity" [TCS – 2014, 18<sup>th</sup> – 21<sup>st</sup> Dec 2014 at NCL & IISER Pune].
4. Presented a poster on Electronic Structure of Five Membered N-Heterocyclic Tetrellylenes, Nhe (E = C - Pb) – An Energy Decomposition Analysis [Tcs – December 2016, at University of Hyderabad].
5. Presented a poster on High Level Quantum Mechanical Study on Molecules Containing Planar Tetracoordinate Centers at IIIT Hyderabad on 2017.

#### **TALKS AT NATIONAL SEMINAR/CONFERENCE**

1. Oral presentation on "Singlet 2-adamantylidene an ambiphilic foiled carbene stabilized by hyperconjugation" [RAC – 2015, 3<sup>rd</sup> Nov 2015 at Central University of Kerala, Kasaragod].