

CURRICULUM VITAE

Dr. Rositha Kuniyil

Date of Birth: 16/07/1990
Place of Birth: Kerala, India
Current Address: Department of Chemistry,
Indian Institute of Technology Palakkad (IIT-PKD),
Ahalia Integrated Campus,
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EDUCATION

- 2013-2017**
Tarragona, Spain
ICIQ (Institut Català d'Investigació Química), Barcelona Institute of Science and Technology (BIST), Tarragona, Spain
PhD in theoretical and computational chemistry with Excellent Cum Laude
- July. 2016**
Tarragona, Spain
Universitat Rovira i Virgili, Tarragona, Spain
Diploma in teaching assistantship
- 2011-2013**
Mumbai, India
Indian Institute of Technology Bombay (IITB), Mumbai, India
Master degree in chemistry
- 2008-2011**
Kerala, India
Farook College, University of Calicut, Kerala, India
Bachelor degree in chemistry

PROFESSIONAL EXPERIENCE

- June 2021- Present**
Assistant Professor – IIT Palakkad
- Nov 2020- June 2021**
Pittsburgh, USA
Postdoctoral Researcher – University of Pittsburgh
Advisor : Prof. Peng Liu
Computational mechanistic studies on transition metal catalyzed reactions
- June 2018- Oct.2020**
Göttingen, Germany
Postdoctoral Researcher – Georg-August Universität Göttingen
Advisor : Prof. Lutz Ackermann
Computational mechanistic studies on C-H activation reactions
- Oct. 2013- Nov. 2017**
Tarragona, Spain
PhD in Theoretical and Computational Chemistry – ICIQ (BIST)
Advisor : Prof. Feliu Maseras
Computational mechanistic studies on the transition metal catalyzed activation of CO₂
- Sep. 2015- Dec. 2015**
Edinburgh, UK
Short Term Scientific Mission (COST Action CM-1205 CARISMA) – Heriot-Watt University
Advisor : Prof. Stuart Macgregor
Computational mechanistic studies on ruthenium catalyzed C-H Activation
Benchmark studies on DLPNO-CCSD(T) method

July. 2013- Sep. 2013
Mumbai, India

Research Assistant- IIT Bombay
Advisor : Prof. Raghavan B. Sunoj
Computational studies on transition states models for stereoselective bond formation in asymmetric organocatalytic reactions

May. 2012- June. 2013
Mumbai, India

Master Thesis in Computational Chemistry – IIT Bombay
Advisor : Prof. Raghavan B. Sunoj
Computational mechanistic studies on enantioselective NHC catalyzed Stetter reaction

PUBLICATIONS

1. Zhang, S. K.; Vecchio, A. D.; **Kuniyil, R.**; Messinis, A. M.; Lin, Z.; Ackermann, L. "Electrocatalytic C–H phosphorylation through nickel (III/IV/II) catalysis" *Chem.* **2021**, *7*, 1379-1392

impact factor: 19.735

2. Shen, Z.; Maksso, I.; **Kuniyil, R.**; Rogge, T.; Ackermann, L. "Rhodaelectro-catalyzed chemo-divergent C–H activations with alkylidene cyclopropanes for selective cyclopropylations" *Chem. Commun.* **2021**, *57*, 3668-3671

impact factor: 5.996

3. Liu, J. B.; Wang, X.; Messinis, A. M.; Liu, X. J.; **Kuniyil, R.**; Chen, D. Z.; Ackermann, L. "Understanding the unique reactivity patterns of nickel/JoSPOphos manifold in the nickel-catalyzed enantioselective C–H cyclization of imidazoles" *Chem. Sci.* **2021**, *12*, 718-729

impact factor: 9.346

4. Wang, W.; Wu, J.; **Kuniyil, R.**; Lima, R. N.; Ackermann, L. "Peptide Late-Stage Diversifications by Rhodium-Catalyzed Tryptophan C7 Amidation" *Chem.* **2020**, *6*, 3428-3439

impact factor: 19.735

5. Yang, L.; Jei, B. B.; Scheremetjew, A.; **Kuniyil, R.**; Ackermann, L. "Electrochemical B–H Nitrogenation: Access to Amino Acid and BODIPY-Labeled nido-Carboranes" *Angew. Chem. Int. Ed.* **2020**, *60*, 1482-1487

impact factor: 12.959

6. Choi, I.; Müller, V.; Wang, Y.; Xue, K.; **Kuniyil, R.**; Andreas, L. B.; Karius, V.; Alauzun, J. G.; Ackermann, L. "Recyclable Ruthenium Catalyst for Distal meta-C–H Activation" *Chem. Eur. J.* **2020**, *26*, 15290

impact factor: 4.857

7. Rogge, T.; Oliveira, J.; **Kuniyil, R.**; Hu, L.; Ackermann, L. "Reactivity-Controlling Factors in Carboxylate-Assisted C–H Activation under 4d and 3d Transition Metal Catalysis" *ACS Catal.* **2020**, *10*, 10551-10558

impact factor: 12.35

8. Korvorapun, K.; Struwe, J.; **Kuniyil, R.**; Zangarelli, A.; Casnati, A.; Waeterschoot, M.; Ackermann, L. "Photo-Induced Ruthenium-Catalyzed C–H Arylations at Room Temperature" *Angew. Chem. Int. Ed.* **2020**, *59*, 18103-18109

impact factor: 12.959

9. Bu, Q.;* **Kuniyil, R.**;* Zhigao, S.; Gońka, E.; Ackermann, L. "Insights into Ruthenium(II/IV)-Catalyzed Distal C–H Oxygenation by Weak Coordination" *Chem. Eur. J.* **2020**, *26*, 16450 (*contributed equally)

impact factor: 4.857

10. Yang, L.; Steinbock, R.; Scheremetjew, A.; **Kuniyil, R.**; Finger, L. H.; Messinis, A.; Ackermann, L. "Aza-Ruthena(II)-Bicyclo-[3.2.0]-Heptadiene: Key Intermediate for Ruthenaelectro(II/III/I)-Catalyzed Alkyne Annulations" *Angew. Chem. Int. Ed.* **2020**, *59*, 11130-11135

impact factor: 12.959

11. Liang, Y.-F.; Yang, L.; Jei, B. B.; **Kuniyil, R.**; Ackermann, L. "Regioselective B(3,4)-H Arylation of o-Carboranes by Weak Amide Coordination at Room Temperature" *Chem. Sci.* **2020**, *11*, 10764-10769
impact factor: 9.346
12. Zhu, C.; **Kuniyil, R.**; Jei, B. B.; Ackermann, L. "Domino C-H Activation/Directing Group Migration/Alkyne Annulation: Unique Selectivity by d6-Cobalt(III) Catalysts" *ACS Catal.* **2020**, *10*, 4444-4450
impact factor: 12.35
13. Massignan, L.; Tan, X.; Meyer, T. H.; **Kuniyil, R.**; Messinis, A. M.; Ackermann, L. "C-H Oxygenation Reactions Enabled by Dual Catalysis with Electrogenerated Hypervalent Iodine Species and Ruthenium Complexes" *Angew. Chem. Int. Ed.* **2020**, *59*, 3184-3189
impact factor: 12.959
14. Korvorapun, K.; **Kuniyil, R.**; Ackermann, L. "Late-Stage Diversification by Selectivity Switch in meta-C-H Activation: Evidence for Singlet Stabilization" *ACS Catal.* **2020**, *10*, 435-440
impact factor: 12.35
15. Xu, Z.; Huang, Z.; Li, Y.; **Kuniyil, R.**; Zhang, C.; Ackermann, L.; Ruan, Z. "Catalyst-Free, Direct Electrochemical Synthesis of Annulated Medium-Sized Lactams through C-C Bond Cleavage" *Green Chem.* **2020**, *22*, 1099-1104
impact factor: 9.405
16. Gońka, E.; Yang, L.; Steinbock, R.; Pescioli, F.; **Kuniyil, R.**; Ackermann, L. "π-Extended Polyaromatic Hydrocarbons by Sustainable Alkyne Annulations through Double C-H/N-H Activation" *Chem. Eur. J.* **2019**, *25*, 16246-16250
impact factor: 4.857
17. Kong, W.-J.; Finger, L. H.; Messinis, A. M.; **Kuniyil, R.**; Oliveira, J. C. A.; Ackermann, L. "Flow Rhodoelectro-Catalyzed Alkyne Annulations by Versatile C-H Activation: Mechanistic Support for Rhodium(III/IV)" *J. Am. Chem. Soc.* **2019**, *141*, 17198-17206
impact factor: 14.612
18. Virelli, M.; Wang, W.; **Kuniyil, R.**; Wu, J.; Zanoni, G.; Fernandez, A.; Scott, J.; Vendrel, M.; Ackermann, L. "BODIPY-Labeled Cyclobutanes by Secondary C(sp³)-H Arylations for Live-Cell Imaging" *Chem. Eur. J.* **2019**, *25*, 12712-12718
impact factor: 4.857
19. Zhu, C.; **Kuniyil, R.**; Ackermann, L.; "Manganese(I)-Catalyzed C-H Activation/Diels-Alder/retro-Diels-Alder Domino Alkyne Annulation by Transformable Pyridines" *Angew. Chem. Int. Ed.* **2019**, *58*, 5338-5342
impact factor: 12.959
20. Lorion, M. M.; Kaplaneris, N.; Son, J.; **Kuniyil, R.**; Ackermann, L. "Late-Stage Peptide Diversification by Cobalt-Catalyzed C-H Activation: Sequential Multicatalysis for Stapled Peptides" *Angew. Chem. Int. Ed.* **2019**, *58*, 1684-1702
impact factor: 12.959
21. Dias, G. G.; Rogge, T.; **Kuniyil, R.**; Jacob, C.; Menna-Barreto, R. F. S.; da Silva Júnior, E. N.; Ackermann, L. "Ruthenium-catalyzed C-H oxygenation of quinones by weak O-coordination for potent trypanocidal agents" *Chem. Commun.* **2018**, *54*, 12840-12843
impact factor: 5.996
22. Simonetti, M.; **Kuniyil, R.**; Macgregor, S.; Larrosa, I. "Benzoate cyclometalation enables oxidative addition of haloarenes at a Ru (II) center" *J. Am. Chem. Soc.* **2018**, *140*, 11836-11847
impact factor: 14.612

23. Guo, W.; **Kuniyil, R.**; Gómez, J. E.; Maseras, F.; Kleij, A. W. A "Domino Process toward Functionally Dense Quaternary Carbons through Pd-Catalyzed Decarboxylative C(sp³)-C(sp³) Bond Formation" *J. Am. Chem. Soc.* **2018**, *140*, 3981-3987 (front cover page)

impact factor: 14.612

24. **Kuniyil, R.**; Maseras, F. "Computational study on the mechanism of the reaction of carbon dioxide with siloxy silanes" *Theor. Chem. Acc.* **2017**, *136*, 1-7

impact factor: 2.233

25. Guo, W.; Rodríguez, L. M.; **Kuniyil, R.**; Martin, E.; Adan, E. C. E.; Maseras, F.; Kleij, A. W. "Stereoselective and Versatile Preparation of Tri- and Tetrasubstituted Allylic Amine Scaffolds under Mild Conditions" *J. Am. Chem. Soc.* **2016**, *138*, 11970-11978

impact factor: 14.612

26. **Kuniyil, R.**; Sunoj, R. B. "N-Heterocyclic Carbene Catalyzed Asymmetric Intermolecular Stetter Reaction: Origin of Enantioselectivity and Role of Counterions" *Org. Lett.* **2013**, *15*, 5040-5043

impact factor: 6.555

POSTERS/ORAL PRESENTATION

- Beilstein Organic Chemistry Online Symposium, Sep.2020 (participant)
- 1st Virtual International symposium on C-H Activation, July 2020 (participant)
- "Palladium catalyzed conversion of cyclic vinyl carbonates to allylic amines: A DFT study", European Conference on Theoretical and Computational Chemistry (EUCCO-TCC), Barcelona, Sep. 2017 (poster)
- "Selective transformation of cyclic vinyl carbonates to allylic amines and aldehydes: A DFT study", The World Association of Theoretical and Computational Chemists (WATOC) conference, Munich, Aug. 2017 (poster)
- "Mechanistic insights into the palladium catalyzed stereoselective formation of allylic amines", XXXII annual meeting of reference network of R+D+i on theoretical and computational chemistry, Tarragona, July 2017 (oral)
- "Mechanistic insights into the carboxylation of α -siloxy silane-A DFT study", CARISMA-COST meeting, Lisbon, March 2017 (oral)
- "Mechanistic insights into the carboxylation of α -siloxy silane-A DFT study" 10th congress on electronic structure: principles and applications (ESPA), Castellon, June 2016 (poster)
 - "Salient role of counterion in the carboxylation of α -siloxy silanes via brook rearrangement - A DFT study", CO₂ catalysis conference, Lisbon, April 2016 (poster)
- "Salient role of AlEt₃ in the allene carboxylation reaction - A DFT study", XXI international conference in organometallic chemistry (EuCOMC), Bratislava, July 2015 (poster)
- XXXI annual meeting of reference network of R+D+i on theoretical and computational chemistry, Girona, June 2015 (participant)
- "Salient role of AlEt₃ in the allene carboxylation reaction- A DFT study" CARISMA-III meeting, Tarragona, March 2015 (poster)
- "Unusual ligand rearrangement in Pd-pincer complex- A case study with allene carboxylation reaction employing DFT method", 50th symposium on theoretical chemistry, Vienna, Sep. 2014 (poster)
- "Mechanistic insights into the allene carboxylation reaction from DFT calculations", VIIth international school on organometallic chemistry, Barcelona, June 2014 (poster)
- DETIC (dialogue between experiment and theory in inorganic chemistry) meeting, Tarragona, Nov. 2013 (participant)
- 3rd Indo-German conference on modeling chemical and biological (re) activity, Mohali, Feb. 2013 (participant)

TEACHING ASSISTANSHIP

Teaching assistantship for master's students on 'introduction to computational chemistry' course, Universitat Rovira i Virgili, Tarragona, Spain (2015-2017)

AWARDS AND SCHOLARSHIPS

- Awarded Formación del Profesorado Universitario, FPU (FPU13/04581) PhD grant from Ministry of Spain for promising future university professors (Nov. 2013 - Nov.2017)
- Awarded diploma in teaching assistantship from Universitat Rovira i Virgili, Tarragona, Spain (2016)
- Awarded CARISMA-COST short term scientific mission fellowship (COST Action CM-1205 CARISMA) for conducting research in an international university from European Union CARISMA-COST organisation (Sept. 2015 - Dec. 2015)
- Awarded highest grade in the first stage and second stage master thesis presentation at IIT Bombay (2012- 2013)
- Selected to participate in the 'magic in chemistry' exhibition as a part of tech-fest at IIT Bombay (2013)
- Awarded Bristol-Mayers-Squibb scholarship from IIT Bombay for academic excellence (Jul. 2012 - May 2013)
- Awarded merit-cum-means scholarship from IIT Bombay for academic support (July 2011 - May 2012)
- Qualified highly competitive all India level IIT JAM (Joint Admission for MSc) for the admission to master's course (2011)
- Selected to participate in the 'chem-eleon2011' exhibition conducted by Farook College, Kerala (2011)
- 2nd batch topper from department of chemistry, Farook College, Kerala (2008-2011)
- Awarded Paloli committee scholarship by government of Kerala for academic excellence (2009-2011)

EXTERNALLY FUNDED PROJECTS

1. Research Assistant -12CSIR004:

Title: Computational studies on transition state models for stereoselective bond formation in asymmetric organocatalytic reactions

Duration: 1-07-2013 to 30-09-2013

Sponsor: Industrial Research and Consultancy Centre, IIT Bombay

Value: 30000 INR

Supervisor: Prof. Raghavan B. Sunoj, IIT Bombay, India

2. CARISMA COST Action CM-1205:

Title: Study of the structure and dynamic behavior of CO₂ as a ligand

Duration: 16-09-2015 to 15-12-2015

Sponsor: CARISMA-COST organization, European Union

Value: 1.6 lakh INR

Supervisor: Prof. Stuart Macgregor, Heriot-watt university, Scotland

3. Formación del Profesorado Universitario, FPU (FPU13/04581) PhD Grant:

Title: Computational mechanistic studies on the transition metal catalyzed activation of CO₂

Duration: 20-09-2013 to 20-09-2017

Sponsor: Ministry of Spain

Value: 35.55 lakh INR

Supervisor: Prof. Feliu Maseras, ICIQ, Spain

SKILLS

- Programming: C, Fortran77, Python
- Softwares and Tools: Gauss view, Molden, VMD, Acuchem, Monte Carlo, Gaussian09, Gaussian16, CP2K, ORKA, NBO, QChem, EDA AIM, Copasi, NCI, Chemcraft and CYL view
- Operating Systems: Linux, Windows
- Language Skills: English, Hindi, and Malayalam (Fluent), Spanish and German (basics)