

# K. R. Justin Thomas, PhD

**Professor, Department of Chemistry  
Indian Institute of Technology Roorkee  
Roorkee – 247667**

## Professional Experience

**PROFESSOR** • INDIAN INSTITUTE OF TECHNOLOGY ROORKEE • DEC 21, 2018 – TO PRESENT

**HEAD** • DEPARTMENT OF CHEMISTRY, INDIAN INSTITUTE OF TECHNOLOGY ROORKEE • APR 01, 2019 – APR 17, 2022

**ASSOCIATE PROFESSOR** • INDIAN INSTITUTE OF TECHNOLOGY ROORKEE • OCT 23, 2012 – DEC 21, 2018

**ASSISTANT PROFESSOR** • INDIAN INSTITUTE OF TECHNOLOGY ROORKEE • MAR 18, 2006 – OCT 22, 2012

**POST-DOCTORAL FELLOW** • ACADEMIA SINICA, TAIPEI, TAIWAN • OCT 1997 – APR 2003 & JUNE 2004 – FEB 2006 (Supervisor: Prof. J. T. Lin)

**POST-DOCTORAL FELLOW** • UNIVERSITY OF MASSACHUSETTS, AMHERST, USA • MAY 2003–MAY 2004 (Supervisor: Prof. S. Thayumanavan)

## Honors

**EDITOR** • ANALYTICAL CHEMISTRY LETTERS, TAYLOR & FRANCIS • SEP 2020 – AUG 2023

**ASSOCIATE EDITOR** • JOURNAL OF INFORMATION DISPLAY, TAYLOR & FRANCIS • JAN 2020 – DEC 2022

**ACADEMIC EDITOR** • INTERNATIONAL JOURNAL OF PHOTOENERGY, HINDAWI • JAN 2016 – PRESENT

**GUEST EDITOR** • SPECIAL ISSUE OF MATERIALS: ADVANCED ORGANIC MATERIALS FOR PHOTOVOLTAIC APPLICATIONS • MAY 2022 –MAR 2023

## Education

**PH.D. • 1995 • INDIAN INSTITUTE OF TECHNOLOGY KANPUR**  
SPECIALIZATION: INORGANIC HETEROCYCLES & COORDINATION CHEMISTRY  
SUPERVISOR: PROF. V. CHANDRASEKHAR

**M.SC. • 1990 • AMERICAN COLLEGE MADURAI**  
SPECIALIZATION: CHEMISTRY; MARKS: 71%

**B.SC. • 1988 • MADURAI KAMARAJ UNIVERSITY**  
SPECIALIZATION: CHEMISTRY, PHYSICS & MATHEMATICS; MARKS: 85.7%

## Publications (last five years)

1. Phenanthroimidazole substituted imidazo[1,2-a]pyridine derivatives for deep-blue electroluminescence with CIE<sub>y</sub> ~ 0.08, Anupriya, K. R. J. Thomas, M. R. Nagar, Shahnawaz, J.-H. Jou, *J. Photochem. PhotoBiol. A: Chem.*, **2022**, *423*, 113600. (DOI: 10.1016/j.jphotochem.2021.113600)
2. Imidazo[1,2-a]pyridine based deep-blue emitter: effect of donor on the optoelectronic properties, Anupriya, K. R. J. Thomas, M. R. Nagar, Shahnawaz, J.-H. Jou, *J. Mater. Sci.: Mater. Electron.*, **2021**, *32*, 26838-26850. (DOI: 10.1007/s10854-021-07060-5)
3. Effect of Cyano on the Functional Properties of Phenanthroimidazole-Substituted Carbazole Derivatives, A. Sharma, K. R. J. Thomas, K. K. Kesavan, I. Siddiqui, M. R. Nagar, J.-H. Jou, *ACS Appl. Electron. Mater.*, **2021**, *3*, 3876-3888 (DOI: 10.1021/acsaelm.1c00482)
4. Phenanthroimidazole-based bipolar carbazoles featuring cyano substituents to realize efficient deep-blue electroluminescence with an external quantum efficiency of nearly 6%, A. Sharma, K. R. J. Thomas, M. R. Nagar, J.-H. Jou, *Mater. Adv.*, **2021**, *2*, 6326-6338 (DOI: 10.1039/D1MA00604E)
5. Effect of positional isomerism on the functional properties of carbazole-phenanthroimidazole-triphenylamine triads, A. Sharma, K. R. J. Thomas, K. K. Kesavan, I. Siddiqui, M. R. Nagar, J.-H. Jou, *Dyes Pigm.*, **2021**, *196*, 109744 (DOI: 10.1016/j.dyepig.2021.109744)
6. Experimental and DFT studies of gadolinium decorated graphene oxide materials for their redox properties and as a corrosion inhibition barrier layer on Mg AZ13 alloy in a 3.5% NaCl environment, N. Palaniappan, I. S. Cole, K. Damodaran, A. E. Kuznetsov, K. R. J. Thomas, K. Balasubramanian, S. Manickam, *RSC Adv.*, **2021**, *11*, 22095-22105 (DOI: 10.1039/d1ra03495b)
7. Dithienopyrrole-based dianchoring dyes: Effect of molecular design and donors on the optical and photovoltaic properties, S. Kumar, K. R. J. Thomas, M. S. Fan, K. C. Ho, *J. Lumin.*, **2021**, *230*, 117727 (DOI: 10.1016/j.jlumin.2020.117727)
8. Tuning photophysical and electroluminescent properties of phenanthroimidazole decorated carbazoles with donor and acceptor units: beneficial role of cyano substitution, A. Sharma, R. Balasaravanan, K. R. J. Thomas, M. Ram, D. K. Dubey, R. A. K. Yadav, J.-H. Jou, *Dyes Pigm.*, **2021**, *184*, 108830 (DOI: 10.1016/j.dyepig.2020.108830).
9. Facile Thiol-Ene Click Protocol Using Benzil as Sensitizer and White LED as Light Source, A. Das, K. R. J. Thomas, *Eur. J. Org. Chem.*, **2020**, 7214-7218 (DOI: 10.1002/ejoc.202001275)
10. Light promoted synthesis of quinoxalines and imidazo[1,2-a]pyridines via oxybromination from alkynes and alkenes, A. Das, K. R. J. Thomas, *Asian J. Org. Chem.*, **2020**, *9*, 1820-1825 (DOI: 10.1002/ajoc.202000388)
11. Fine-tuning the physicochemical and electroluminescence properties of multiply-substituted bipolar carbazoles by functional group juggling, R. K. Konidena, K. R. J. Thomas, D. K. Dubey, S. Sahoo, J.-H. Jou, *ChemPhotoChem*, **2020**, *4*, 5364-5375 (DOI: 10.1002/cptc.202000172)
12. Effect of auxiliary donors and position of benzothiadiazole on the optical and photovoltaic properties of dithieno[3,2-b:2',3'-d]pyrrole-based sensitizers, S. Kumar, K. R. J. Thomas, C.-T. Li, M.-S. Fan, K.-C. Ho, *Solar Energy*, **2020**, *208*, 539-547 (DOI: 10.1016/j.solener.2020.08.001)
13. Synthesis and characterization of multi-substituted carbazole derivatives exhibiting aggregation-induced emission for OLED applications, A. Sharma, D. Saklani, K. R. J. Thomas, Shahnawaz, S. S. Swayamprabha, J.-H. Jou, *Org. Electron.*, **2020**, *86*, 105864 (DOI: 10.1016/j.orgel.2020.105864)
14. Asymmetrically 2,7-difunctionalized carbazole-based donor-acceptor hybrids for deep blue electroluminescence applications, V. Joseph, K. R. J. Thomas, S. Sahoo, M. Singh, J.-H. Jou, *Opt. Mater.*, **2020**, *108*, 110159, (DOI: 10.1016/j.optmat.2020.110159)
15. Experimental and DFT studies of porous carbon covalently functionalized by polyaniline as a corrosion inhibition barrier on nickel-based alloys in acidic media, N. Palaniappan, I. S. Cole,

- K. Damodaran, A. E. Kuznetsov, K. R. J. Thomas, K. Balasubramanian, *RSC Adv.*, **2020**, *10*, 12151-12165 (DOI: 10.1039/d0ra00593b)
16. Experimental and DFT studies on the ultrasonic energy-assisted extraction of the phytochemicals of *Catharanthus roseus* as green corrosion inhibitors for mild steel in NaCl medium, N. Palaniappan, I. S. Cole, F. Caballero-Briones, S. Manickam, K. R. J. Thomas, D. Santos, *RSC Adv.*, **2020**, *10*, 5399-5411 (DOI: 10.1039/c9ra08971c)
  17. Experimental and DFT studies of carbon nanotubes covalently functionalized with an imidazole derivative for electrochemical stability and green corrosion inhibition as a barrier layer on the nickel alloy surface in a sulphuric acidic medium, N. Palaniappan, I. S. Cole, A. E. Kuznetsov, K. R. J. Thomas, *RSC Adv.*, **2019**, *9*, 38677-38686 (DOI: 10.1039/c9ra08123b)
  18. Experimental and computational studies of a graphene oxide barrier layer covalently functionalized with amino acids on Mg AZ13 alloy in salt medium, N. Palaniappan, I. S. Cole, A. E. Kuznetsov, K. Balasubramanian, K. R. J. Thomas, *RSC Adv.*, **2019**, *9*, 32441-32447 (DOI: 10.1039/c9ra06549k)
  19. Fine tuning the absorption and photovoltaic properties of benzothiadiazole dyes by donor-acceptor interaction alternation via methyl position, A. Pathak, T. Tomer, K. R. J. Thomas, M.-S. Fan, K.-C. Ho, *Electrochim. Acta*, **2019**, *304*, 1-10. (DOI: 10.1016/j.electacta.2019.02.077)
  20. Triazine-branched mono- and dianchoring organic dyes: Effect of acceptor arms on optical and photovoltaic properties, K.R.J. Thomas, A. Venkateswararao, R. Balasaravanan, C.-T. Li, K.-C. Ho, *Dyes Pigm.*, **2019**, *165*, 182-192. (DOI: 10.1016/j.dyepig.2019.02.013)
  21. Design-to-Device Approach Affords Panchromatic Co-Sensitized Solar Cells, C. B. Cooper, E. J. Beard, Álvaro Vázquez-Mayagoitia, L. Stan, G. B. G. Stenning, D. W. Nye, J. A. Vigil, T. Tomar, J. Jia, G. B. Bodedla, S. Chen, L. Gallego, S. Franco, A. Carella, K. R. J. Thomas, S.Xue, X. Zhu, J. M. Cole, *Adv. Energy Mater.*, **2019**, *9* 1802820 (DOI: 10.1002/aenm.201802820)
  22. Polarity tuning of fluorene derivatives by chromophores to achieve efficient blue electroluminescent materials, K. R. J. Thomas, A. Venkateswararao, V. Joseph, S. Kumar, J.-H. Jou, *Org. Electron.*, **2019**, *64*, 266-273. (DOI: 10.1016/j.orgel.2018.10.029)
  23. Effect of electron rich  $\pi$ -linkers on the functional properties of dyes featuring dithieno[3,2-b:2',3'-d]pyrrole donor, S. Kumar, K. R. J. Thomas, C.-T. Li, K.-C. Ho, *Dyes Pigm.*, **2019**, *160*, 614-623. (DOI: 10.1016/j.dyepig.2018.08.035)
  24. Vinyl-Linked Cyanocarbazole-Based Emitters: Effect of Conjugation and Terminal Chromophores on the Photophysical and Electroluminescent Properties, V. Joseph, K. R. J. Thomas, S. Sahoo, M. Singh, J.-H. Jou, *ACS Omega*, **2018**, *3*, 16477-16488. (DOI: 10.1021/acsomega.8b02198)
  25. Tuning the photophysical and electroluminescence properties in asymmetrically tetrasubstituted bipolar carbazoles by functional group disposition, R. K. Konidena, K. R. J. Thomas, A. Pathak, D. K. Dubey, S. Sahoo, J.-H. Jou, *ACS Appl. Mater. Interfaces*, **2018**, *10*, 24013-24027. (DOI: 10.1021/acsmi.8b04566)
  26. Enabling a 6.5% external quantum efficiency deep-blue organic light-emitting diode with a solution-processable carbazole based emitter, J.-H. Jou, J.-L. Li, S. Sahoo, D. K. Dubey, R. A. K. Yadav, V. Joseph, K. R. J. Thomas, C.-W. Wang, J. Jayakumar, C.-H. Cheng, *J. Phys. Chem. C.*, **2018**, *42*, 24295-24303. (DOI: 10.1021/acs.jpcc.8b07641)
  27. Wide color gamut deep-blue OLED architecture for display application, D. K. Dubey, R. K. Konidena, S. Sahoo, R. A. K. Yadav, S. S. Swayamprabha, K. R. J. Thomas, J.-H. Jou, *ECS Trans.*, **2018**, *85*, 33-39. (DOI: 10.1149/08507.0033ecst)
  28. Synthesis and characterization of naphthalimide-based dyes for dye sensitized solar cells, A. Saini, K. R. J. Thomas, Y.-J. Huang, K.-C. Ho, *J. Mater. Sci. Mater. Electron.*, **2018**, *29*, 16565-16580. (DOI: 10.1007/s10854-018-9750-4)
  29. Cyano-functionalized carbazole substituted pyrene derivatives for promising organic light-emitting diodes, V. Joseph, K. R. J. Thomas, S. Sahoo, M. Singh, J.-H. Jou, *Dyes Pigm.*, **2018**, *158*, 295-305. (DOI: 10.1016/j.dyepig.2018.05.038)

30. Tetra-substituted dipolar carbazoles: Tuning optical and electroluminescence properties by linkage variation, V. Joseph, K. R. J. Thomas, W. Y. Yang, R. A. K. Yadav, D. K. Dubey, J.-H. Jou, *Asian J. Org. Chem.*, **2018**, *7*, 1654-1666. (DOI: 10.1002/ajoc.201800248)
31. Simple carbazole based deep-blue emitters: The effect of spacer, linkage and end-capping cyano group on the photophysical and electroluminescent properties, V. Joseph, K. R. J. Thomas, S. Sahoo, M. Singh, J.-H. Jou, *Dyes Pigm.*, **2018**, *151*, 310-320. (DOI: 10.1016/j.dyepig.2017.12.061)
32. Highly efficient deep-blue organic light emitting diode with a carbazole based fluorescent emitter, S. Sahoo, D. K. Dubey, M. Singh, V. Joseph, K. R. J. Thomas, J.-H. Jou, *Jpn. J. Appl. Phys.*, **2018**, *57*, 04FL08 (DOI: 10.7567/JJAP.57.04FL08)
33. T-Shaped Benzimidazole Derivatives as Blue-Emitting Materials: Role of C2 Substituents on Photophysical Properties, K. R. J. Thomas and G. B. Bodedla, *Asian J. Org. Chem.*, **2018**, *7*, 729-738. (DOI: 10.1002/ajoc.201800003).
34. Manipulation of donor-acceptor interactions in carbazole-based emitters by chromophore choice to achieve near-UV emission, V. Joseph, K. R. J. Thomas, M. Singh, S. Sahoo, J.-H. Jou, *Eur. J. Org. Chem.*, **2017**, 6660-6670. (DOI: 10.1002/ejoc.201701285)
35. Fine-Tuning of Photophysical and Electroluminescence Properties of Benzothiadiazole-Based Emitters by Methyl Substitution, A. Pathak, K. R. J. Thomas, M. Singh, J.-H. Jou, *J. Org. Chem.*, **2017**, *82*, 11512-11523. (DOI: 10.1021/acs.joc.7b02127)
36. New Molecular Design Based on Hybridized Local and Charge Transfer Fluorescence for Highly Efficient (> 6%) Deep-Blue Organic Light Emitting Diodes, R. K. Konidena, K. R. J. Thomas, D. K. Dubey, S. Sahoo, J.-H. Jou, *Chem. Commun.*, **2017**, *53*, 11802-11805. (DOI: 10.1039/C7CC07139F)
37. Effect of electron-deficient linkers on the physical and photovoltaic properties of dithienopyrrole-based organic dyes, S. Kumar, K. R. J. Thomas, C.-T. Li and K.-C. Ho, *J. Mater. Sci. Mater. Electron.*, **2017**, *28*, 18404–18417. (DOI: 10.1007/s10854-017-7787-4)
38. Photophysics, electrochemistry, morphology and bioimaging applications of new 1,8-naphthalimide derivatives containing different chromophores, A. Saini, K. R. J. Thomas, A. Sachdev and P. Gopinath, *Chem. Asian J.* **2017**, *5*, 2612-2622. (DOI: 10.1002/asia.201700968)
39. Star-Shaped Asymmetrically Substituted Blue Emitting Carbazoles: Synthesis, Photophysical, Electrochemical and Theoretical Investigations, R. K. Konidena, K. R. J. Thomas, *ChemistrySelect*, **2017**, *2*, 7514-7524. (DOI: 10.1002/slct.201701336)
40. Effect of Donors on Photophysical, Electrochemical and Photovoltaic Properties of Benzimidazole-Branched Dyes, G. B. Bodedla, K. R. J. Thomas, M.-S. Fan and K.-C. Ho, *ChemistrySelect*, **2017**, *2*, 2807- 2814. (DOI: 10.1002/slct.201700014)
41. Multi-substituted deep-blue emitting carbazoles: a comparative study on photophysical and electroluminescence characteristics, R. K. Konidena, K. R. J. Thomas, S. Sahoo, D. K. Dubey, J.-H. Jou, *J. Mater. Chem. C*, **2017**, *5*, 709-726. (DOI: 10.1039/C6TC04870F)

## Patents (last five years)

1. A method of synthesis of aldehyde and ketones from dicyanovinyl derivatives using photochemical method for C=C bond cleavage of dicyanovinyl derivatives and NBS under light irradiation, K. R. J. Thomas, A. Das, Indian Patent No. 397930.

## Current Strength of Research Group

PhD: 10 (ten)

PDF: 0 (Zero) Vacancy Available

## Sponsored Projects

### Completed

1. Synthesis and characterization of polyaromatic fused quinoxalines as dipolar functional materials, DST, New Delhi (Rs. 2400000, Three years, 2007-2010).
2. New carbazole derivatives for electro-optics, CSIR, New Delhi (Rs. 1300000, Three years, 2007-2010).
3. Synthesis and spectroelectrochemical investigations of organic dyes suitable for dye-sensitized solar cells, MHRD, GOI (Rs. 835000, Two years, 2008-2010)
4. Synthesis and characterization of organic dyes for dye-sensitized solar cells, BASF SE, Germany (€ 30,000; Three years; 2009-2012)
5. New Materials and Methods for the efficient organic photovoltaic devices, DST, New Delhi (Rs. 31,94,000; Two years, 2011-2013)
6. Pyrenoimidazole-based dipolar compounds for photovoltaics, CSIR, New Delhi (Rs. 23,92,000; Three years; 2011-2014)
7. New Materials and Methods for the efficient organic photovoltaic devices (Phase II), DST, New Delhi (Rs. 79,90,000; Three Years, 2015-2018)
8. Organic materials containing heterocyclic building blocks, CSIR, New Delhi (Three Years, Rs. 21,00,000; 2015-2018).
9. Enabling Organic Materials to Harvest Triplet Excitons In Organic Light-Emitting Diodes, CSIR, New Delhi (Three years, 2019-2022, 02(0094)/19)

### In Progress

1. Design and Functional Enrichment of Triplet Harvesting Organic Emitters for OLED, SERB, New Delhi (Three Years, Rs. 6032400; 2019-2022, CRG/2018/003729/OC).
2. Probing the molecular orientation and charge transfer dynamics at interfaces for the design and fabrication of more efficient optoelectronics devices, STARS, Bangalore (Co-PI, Three years, Rs. 9908000, 2019-2022)