# PROFORMA FOR BIO-DATA

1. Name and full correspondence address:

   **Dr. Manoj Vasisht Mane**

   Centre for Nano and Material Sciences, Jain (Deemed-to-be University), Jain Global Campus, Kanakapura, Bangalore, Karnataka, India – 562112

2. Email(s) and contact number(s): manoj.mane@jainuniversity.ac.in

   +91 8308530407

3. Institution: Jain (Deemed-to-be University)

4. Research Interest: Computational Studies on

   - Frustrated Lewis Pairs
   - Metallaphotoredox Catalysis
   - Asymmetric Catalysis
   - Metal−Ligand cooperativity
   - Small Molecules Activation
   - Covalent Organic Framework
   - Selective Ethylene Oligomerization
   - Designing and development of transition metal and transition metal-free catalysed reactions.

5. Gender (M/F): M

6. Ph.D. (2010-2016): Computational Chemistry

   Guide's Name: Dr. Kumar Vanka

   Institute: National Chemical Laboratory, Pune, Maharashtra, India

7. Work experience (in chronological order).

| S. No. | Positions held | Name of the Institute | From | To |
|---|---|---|---|---|
| 1 | Assistant Professor | Center for Nano and Materials Sciences- JAIN University | September 2022 | Current |
| 2 | Postdoctoral Fellow | King Abdullah University of Science and Technology (KAUST), Thuwal, Kingdom of Saudi Arabia | July 2019 | August 2022 |
| 3 | Postdoctoral Fellow | Korea Advanced Institute of Science and Technology (KAIST), Department of Chemistry, Daejeon, South Korea. | August 2016 | June 2019 |
| 4 | Project Assistant | National Chemical Laboratory, Pune, Maharashtra, India | January 2010 | June 2010 |

8. Professional Recognition/Award/Prize/Certificate, Fellowship received by the applicant.

| S. No | Name of Award | Awarding Agency | Year |
|---|---|---|---|
| 1 | CSIR-NET | CSIR-UGC | 2009 |
| 2 | GATE: Chemistry | IIT (Roorkee) | 2009 |

9. **Publications** *(List of papers published in SCI Journals, in year wise descending order).*

| S.No. | Author(s) | Title | Name of Journal | Volume | Page | Year |
|---|---|---|---|---|---|---|
| **51** | Basappa, S.; Prakash, A.; Talekar, S. S.; **Mane, M. V.**; Bose, S. K. | Facile Synthesis of Vinyl Boronate Esters via Dehydrogenative Borylation of Alkenes Enabled by a Co-MOF Catalyst: An Additive-Free Approach | *ACS Catalysis* | 14 | 3065-3073 | 2024 |
| **50** | Talekar, S. S.; Dutta, S.; **Mane, M. V.**; Maity, B. | Visible Light-Induced Photoredox and Copper-Catalyzed C−N Cross-Coupling: A Mechanistic Perspective | *European Journal of Organic Chemistry* | 27 | e202301312 | 2024 |
| **49** | Maurya, A.; Marvaniya, K.; Dobariya, P.; **Mane, M. V.**; Tothadi, S.; Patel, K.; Kushwaha, S. | Biomimetic Helical Hydrogen Bonded Organic Framework Membranes for Efficient Uranium Recovery from Seawater | *Small* | 20 | 2306824 | 2024 |
| **48** | Saini, S.; Gupta, D. K.; Bhawar, R.; Siddiqui, S.; **Mane, M. V.**; Bose, S. B. | Transition-metal-and solvent-free regioselective hydrosilylation of alkenes and allenes enabled by sodium tert-butoxide catalyst | *Green Chemistry* | 25 | 10072-10081 | 2023 |
| **47** | Chavan, S. S.; Jadhav, A. N.; **Mane, M. V.** | Mixed Ligand Copper (I) complexes with alkynyl functionalized iminopyridine and substituted ethynylpyridine ligands: Synthesis, photophysical properties and DFT studies | *Journal of Molecular Structure* | 1294 | 136423 | 2023 |
| **46** | Mohite, S. B.; **Mane, M. V.;** Bera, M.; Karpoormath R. | Palladium-Catalyzed Regiodivergent C-H Olefination of Imidazo [1, 2a] Pyridine Carboxamide and Unactivated Alkenes | *Chemistry–A European Journal* | Early View | e202302759 | 2023 |
| **45** | Sancheti, S. P.; Y Singh, Y.; **Mane, M. V.**; Patil, N. T. | Gold-Catalyzed 1, 2-Dicarbofunctionalization of Alkynes with Organohalides | *Angewandte Chemie International Edition* | 62 | e202310493 | 2023 |
| **44** | Mondal, T.; Biswas, S.; **Mane, M. V.**; Panja, S. S. | Shedding Novel Photophysical Insights Toward Discriminative Detection of Three Toxic Heavy Metal Ions and a | *Journal of Fluorescence* | doi.org/10.1007/s10895-023- | Accepted | 2023 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | | hazard class 1 nitro-explosive By Using a Simple AIEE Active Luminogen | | 03378-x | | |
| **43** | **Mane M. V.**; Maity B.; Cavallo, L. | Mechanistic Study on the Multicomponent C−N Cross Coupling via Dual Copper and Photoredox Catalysis | *ACS Catalysis* | 13 | 6249-6260 | 2023 |
| **42** | Jadhav, A. N.; **Mane, M. V.;** Chavan, S. S. | Mixed Ligand Copper (I) complexes with alkynyl functionalized iminopyridine and substituted ethynylpyridine ligands: Synthesis, photophysical properties and DFT studies | *Journal of Molecular Structure* | *1294* | 136423 | 2023 |
| **41** | Ma, X.; **Mane, M. V.**; Cavallo, L.; Nolan, S. P. | Ruthenium-Catalyzed Regioselective 1,2 Hydrosilylation of N-Heteroarenes | *European Journal of Organic Chemistry* | 26 | e202201466 | 2023 |
| **40** | Mondal, T.; Biswas, S.; **Mane, M. V.**; Panja, S. S. | Deciphering Swift Reversal of Multifaceted Photodynamics of a Novel Pyrene Appended Unsymmetrical Salicylaldehyde Azine Derivative in Aqueous and Protein Environments | *New Journal of Chemistry* | 47 | 5280-5300 | 2023 |
| **39** | Nagtilak, P. J.; **Mane, M. V.**; Prasad, S.; Cavallo, L.; Tantillo, D. J.; Kapur, M. | Merging Rh-catalyzed C-H Functionalization and Cascade Cyclization to Enable Propargylic Alcohols as Three-Carbon Synthons: Experimental and Computational Investigations | *Chemistry–A European Journal* | 29 | e202203055 | **2023** |
| **38** | Maurya, A.; Marvaniya, K.; Dobariya, P.; Chudasama, N.; **Mane, M. V.**; Patel, K.; Kushwaha, S. | Protocol for extraction, characterization, and computational analysis of uranium from seawater | *STAR Protocols* | 4 | 102100 | 2023 |
| **37** | Kaushik, A.; Marvaniya, K.; Kulkarni, Y.; Bhatt, D.; Bhatt, J.; **Mane, M. V.**; Suresh,E.; Tothadi, S.; Patel, K.; Kushwaha, S | Large-area self-standing thin film of porous hydrogen-bonded organic framework for efficient uranium extraction from seawater | *Chem* | *8* | 2749–2765. | 2022 |
| **36** | Chintawar, C. C.; Bhoyare, V. W.; **Mane, M. V.**; Patil, N. T. | Enantioselective Au(I)/Au(III) Redox Catalysis Enabled by Rationally Designed Chiral (P,N)-Ligand | *Journal of the American Chemical Society* | *144* | 7089-7095 | 2022 |
| **35** | Jadhav, A. N.; | Heteroleptic Copper(I) | | | | |

| | | | | | | |
|---|---|---|---|---|---|---|
| | Singh, S. B.; **Mane, M. V.**; Kumbhar, A. S | complexes of bipyridine glycoluril and phosphine ligands: photophysical, biological and computational studies | *Inorganica Chimica Acta* | *538* | 120934 | 2022 |
| **34** | Roy, S.; Mondal, T.; Dey, D.; **Mane, M. V.**; Panja, S. S. | A New Thiophene-Appended Fluorescein-Hydrazone-Based Chromo-Fluorogenic Sensor for the Screening of Hg2+ Ions in Real Water Samples | *ChemistrySelect* | *6* | 10464-10479 | 2021 |
| **33** | Ghosh, A.; Hegde, R. V.; Rode, H. B.; Ambre, R.; **Mane, M. V.**; Patil, S. A.; Sridhar, B.; Dateer, R. B. | Catalyst-and Additive-Free Approach to Constructing Benzo-oxazine, Benzo-oxazepine, and Benzo-oxazocine: O Atom Transfer and C═O, C–N, and C–O Bond Formation at Room Temperature | *Organic Letters* | 23 | 8189-8193 | 2021 |
| **32** | Mondal, T.; Roy, S.; Mondal, I., **Mane, M. V.**; Panja S. S. | Deeper insight into the multifaceted photodynamics of a potential organic functional material emphasizing aggregation induced emission enhancement (AIEE) properties | *J. Photochem. Photobiol. A: Chemistry* | *406* | 112998 | 2021 |
| **31** | Scattolin, T.; Bortolamiol, E.; Palazzolo, S.; Caligiuri, I.; Perin, T.; Canzonieri, V.; Demitri, N.; Rizzolio, F.; Cavallo, L.; Dereli, B.; **Mane, M. V.**; Nolan, S. P.; Visentin, F | The anticancer activity of an air-stable Pd(I)-NHC (NHC = N-heterocyclic carbene) dimer | *Chemical Communication* | *56* | 12238-12241 | 2020 |
| **30** | Kushwaha, S.; **Mane M. V.**; Ravindranathan, S.; Das A | Polymer nanorings with uranium specific clefts for selective recovery of uranium from acidic effluents via reductive adsorption | ACS sensors | *5* | 3254-3263 | 2020 |
| **29** | Shinde, V. S.; **Mane, M. V.**; Cavallo, L.; Rueping, M. | Iridium (I)-Catalyzed Enantioselective Hydroarylation of Alkenes via C-H bond Activation: Experiment and Computation | *Chemistry–A European Journal* | *26* | 8308-8313 | 2020 |
| **28** | Mondal, T.; Mondal, I.; Biswas, S.; **Mane, M.V.**; Panja, S. S. | Mechanistic Insight into Selective Sensing of Hazardous Hg2+ and Explosive Picric Acid by Using a Pyrene- Azine-Hydroxyquinoline Framework in Differential | *ChemistrySelect* | *5* | 9336-9349 | 2020 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | | Media | | | | |
| **27** | Ghosh, A.; **Mane, M. V.**; Rode, H.; Patil, S.; Sridhar, B.; Dateer, R | Catalyst-Free Regioselective (3+ 2)-Cycloadditions of α, β-unsaturated N-arylnitrones with Alkenes to Access Functionalized Isoxazolidines: A DFT Study | *Chemistry – An Asian Journal* | *15* | 899-903 | 2020 |
| **26** | Chintawar, C. C; **Mane M. V.**; Tathe, A. G.; Biswas, S.; Patil, N. T. | Gold-catalyzed cycloisomerization of pyridine-bridged 1, 8-diynes: An expedient access to luminescent cycl [3.2. 2] azines | *Organic Letters* | 21 | 7109–7113 | 2019 |
| **25** | Kim, H. K.; **Mane, M. V.**; Montgomery, J.; Baik, M.-H. | The Mechanism of Copper-Catalyzed Trifunctionalization of Terminal Allenes" | *Chemistry–A European Journal* | *25* | 9456-9463 | 2019 |
| **24** | Bagle, P. N.; **Mane, M. V.**; Sancheti, S. P.; Gade, A. B.; Shaikh, S. R.; Baik, M.-H.; Patil, N. T | Gold(I)-catalyzed –OH Group Assisted C(sp2)–H Alkylation of Enaminones with Diazo Compounds to Access 3-Alkyl Chromones | *Organic Letters* | *21* | 335–339 | 2019 |
| **23** | Lee, H.; **Mane, M. V.**; Ryu, H.; Sahu, D.; Baik, M.-H.; Yi, C. S. | Experimental and Computational Study of the (Z)-Selective Formation of Trisubstituted Olefins and Benzo-Fused Oxacycles from the Ruthenium-Catalyzed Dehydrative C-H Coupling of Phenols with Ketons | *Journal of the American Chemical Society* | *140* | 10289–10296 | 2018 |
| **22** | Dharmapurikar, S. S.; Chithiravel S.; **Mane, M. V.**; Deshmukh, G.; Krishnamoorthy, K. | Dihedral angle control to improve the charge transport properties of conjugated polymers in organic field effect transistors | *Chemical Physics Letters* | *695* | 51-58 | 2018 |
| **21** | Kurogi, T.; **Mane M. V.**, Zheng, S.; Carroll, P. J.; Baik, M.-H.; Mindiola, D. J. | Divergent pathways involving 1,3-dipolar addition and N-N bond splitting of an organic azido across a zirconium methylidene | *Angewandte Chemie International Edition* | *57* | 1978-1981 | 2018 |
| **20** | Solowey, D. P; **Mane, M. V.**; Kurogi, T.; Carroll, P. J.; Manor, B. C.; Baik, M.-H.; Mindiola, D. J. | A new and selective cycle for dehydrogenation of linear and cyclic alkanes under mild conditions using a base metal | *Nature Chemistry* | *9* | 1126-1132 | 2017 |

| | | | | | | |
|---|---|---|---|---|---|---|
| **19** | **Mane, M. V.**; Vanka, K. | Less Frustration, More Activity - Interesting Theoretical Insights into Frustrated Lewis Pairs for Hydrogenation Catalysis | *ChemCatChem* | *9* | 3013-3022 | 2017 |
| **18** | Patel, K.; Deshmukh S.; Bodkhe, D.; **Mane, M. V.**; Kumar Vanka, K.; Shinde, D.; Rajamohanan, P. R.; Nandi, S.; Vaidhyanathan, R.; Chikkali, S. H. | Secondary Interactions Arrest the Hemiaminal Intermediate to Invert the *Modus Operandi* of Schiff Base Reaction: A Route to Benzoxazinones | *The Journal of Organic Chemistry* | *82* | 4342–4351 | 2017 |
| **17** | Parwe, S. P.; Warkad, S. D.; **Mane, M. V.**; Shedage, P.S.; Garnaik, B. | Investigation of the biocompatibility and cytotoxicity associated with ROP initiator and its role in bulk polymerization of l-lactide | *Polymer* | *111* | 244-251 | 2017 |
| **16** | Rizvi, M. A.; **Mane**, **M. V.**; Khuroo, M. A.; Peerzada, G. M. | Computational survey of ligand properties on iron (III)–iron (II) redox potential: exploring natural attenuation of nitroaromatic compounds | *Monatshefte für Chemie-Chemical Monthly* | *148* | 655-668 | 2017 |
| **15** | Gawade, R. L.; Chakravarty, D. K.; Kotmale, A. S.; Sangtani, E.; Joshi, P. V.; Ahmed, A.; **Mane**, **M. V.**; Das, S.; Vanka, K.; Rajamohanan, P. R.; Puranik, V. G.; Gonnade, R. G | Additive Mediated *Syn-Anti* Conformational Tuning at Nucleation to Capture Elusive Polymorphs: Remarkable Role of Extended π-Stacking Interactions in Driving the Self-Assembly | *Crystal Growth & Design* | *16* | 2416–2428 | 2016 |
| **14** | Bagle, P. N.; **Mane**, **M. V.**; Vanka, K.; Shinde, D. R.; Shaikh, S. R.; Gonnade, R. G.; Patil, N. T. | Au (i)/Ag(i) co-operative catalysis: interception of Ag-bound carbocations with α-gold (i) enals in the imino-alkyne cyclizations with N-allenamides | C*hemical Communication* | *52* | 14462-14465 | 2016 |
| **13** | Thangaraj, M.; Bhojgude, S.; **Mane**, **M. V.**; Biju, A. T. | From insertion to multicomponent coupling: temperature dependent reactions of arynes with aliphatic alcohols” | C*hemical Communication* | *52* | 1665-1668 | 2016 |
| **12** | **Mane**, **M. V.**; Rizvi, M.; Vanka, K. | Computational Study of Metal Free Alcohol Dehydrogenation Employing | *The Journal of Organic Chemistry* | *80 (4)* | *2081–2091* | 2015 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | | Frustrated Lewis Pairs | | | | |
| **11** | Shaikh, A. C.; Shalini, S. Vaidhyanathan, R.; **Mane**, **M. V.**; Barui, A. K.; Patra, C. R.; Venkatesh, Y.; Bangal P. R.; Patil, N. T. | Identifying Solid Luminogens through Gold-Catalysed Intramolecular Hydroarylation of Alkynes | *European Journal of Organic Chemistry* | *2015* | 4860–4867 | 2015 |
| **10** | Shinde, V. S.; **Mane**, **M. V.**; Vanka, K.; Mallick, A.; Patil, N. T | Gold(I)/Chiral Brønsted Acid Catalyzed Enantioselective Hydroamination–Hydroarylation of Alkynes: The Effect of a Remote Hydroxyl Group on the Reactivity and Enantioselectivity | *Chemistry – A European Journal* | *21* | 975–979 | 2015 |
| **9** | Rizvi, M.; Zaki, M.; Afzal, M.; **Mane, M.V.**; Kumar, M.; Shah, B. A.; Srivastav, S.; Srikrishna, S.; Peerzada, G. M.; Tabassum, S. | Nuclear blebbing of biologically active organoselenium compound towards human cervical cancer cell (HeLa): In vitro DNA/HAS binding, cleavage and cell imaging studies | *European Journal of Medicinal Chemistry* | *90* | 876–888 | 2015 |
| **8** | Kumar, M.; Kumar, A.; Rizvi, M.; **Mane, M. V.**; Vanka, K.; Taneja, S. C.; Shah, B. A | Synthesis of α,β-Unsaturated δ-Lactones by Vinyl Acetate Mediated Asymmetric Cross-Aldol Reaction of Acetaldehyde: Mechanistic Insights | *European Journal of Organic Chemistry* | *2014* | 5247–5255 | 2014 |
| **7** | Munshi, M. K.; Gade, S. M.; **Mane, M. V.**; Mishra, D.; Pal, S.; Vanka, K.; Rane, V. H.; Kelkar, A. A. | 1,8-Diazabicyclo [5.4.0] undec-7-ene (DBU): A highly efficient catalyst in glycerol carbonate synthesis | *Journal of Molecular Catalysis A: Chemical* | *391* | 144-149 | 2014 |
| **6** | **Mane, M. V.**; Vanka, K. | Proposing Efficient New Pendant Group Polymer Electrolyte Membranes for Fuel Cells: A Computational Study | *Journal of Physical Chemistry C* | *118* | 784–795 | 2014 |
| **5** | Yetra, S. R.; Bhunia, A.; Patra, A.; **Mane, M. V.**; Vanka, K.; Biju, A. T | Enantioselective N-Heterocyclic Carbene-Catalyzed Annulations of 2-Bromoenals with 1,3-Dicarbonyl Compounds and Enamines *via* Chiral α,β-Unsaturated Acylazoliums | *Advanced Synthesis & Catalysis* | *355* | 1089-1097 | 2013 |
| **4** | Ghatak, K.; **Mane,** | Metal or Nonmetal Cooperation with a Phenyl | | | | |

| | | | | | | |
|---|---|---|---|---|---|---|
| | **M. V.**; Vanka, K. | Group: Route to Catalysis? A Computational Investigation | *ACS Catalysis* | *3* | 920-927 | 2013 |
| **3** | Tayade, K. N.; **Mane, M. V.**; Sen, S.; Murthy, C.N.; Tembe, G. L; Pillai, S. M.; Vanka, K.; Mukherjee, S. | A catalytic and DFT study of selective ethylene oligomerization by nickel(II) oxime-based complexes | *Journal of Molecular Catalysis A: Chemical* | *366* | 238-246 | 2013 |
| **2** | Kandambeth, S.; Mallick, A.; Lukose, B.; **Mane, M. V.**; Heine, T.; Banerjee, R. | Construction of Crystalline 2D Covalent Organic Frameworks with Remarkable Chemical (Acid/Base) Stability via a Combined Reversible and Irreversible Route | *Journal of the American Chemical Society* | *134* | 19524-19527 | 2012 |
| **1** | **Mane, M. V.**; Venkatnathan, A.; Ghatak, K.; Vanka, K. | Exploring the Potential of Doped Zero-Dimensional Cages for Proton Transfer in Fuel Cells: A Computational Study | *Journal of Physical Chemistry B* | *116* | 9803–9811 | 2012 |

10. Detail of patents.

| S.No | Patent Title | Name of Applicant(s) | Patent No. | Award Date | Agency/Country | Status |
|---|---|---|---|---|---|---|
| | | | | | | |
| | | | | | | |

14. Books/Reports/Chapters/General articles etc.

| S.No | Title | Author's Name | Publisher | Year of Publication |
|---|---|---|---|---|
| 1 | Schrock vs. Fischer Carbenes: A Quantum Chemical Perspective | Won, J.; Jung, H.; **Mane, M. V.**; Heo, J.; Kwon, S.; Baik, M.-H | *Advance Inorganic Chemistry* | 2019 |
| | | | | |