

DATTA MARKAD, *Ph.D.*

Synthetic Chemist

Materials Innovation Factory | Department of Chemistry
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[Webpage Link](#)

Research Interest:

Multifunctional Porous Materials | Organic and Inorganic Synthesis | Metal-organic Frameworks (MOFs) | Heterogeneous Catalysis | Chemical Separation | X-ray Crystallography | Supramolecular Chemistry | Crystal Structure Determination.

Research Experience/ Academic Qualification:

09/2019 – Present **Research Associate**

- Materials Innovation Factory, University of Liverpool, United Kingdom.
- Project: [DYNAPORE](#) (*Dynamic responsive porous crystals*) a European Research Council Advanced Grant project
- Adviser: **Prof. Matthew J. Rosseinsky**

01/2014 – 05/2019 **Doctor of Philosophy in Chemical Sciences**

- Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, India.
- One-year course work with CPI **9.2/10**
- Thesis Title: “*Flexible and Semirigid Bis(tridentate) Pyridyl, Pyridyl-Amide and Pyridyl-Carboxylate Ligands and their Metal-Organic Coordination Networks: Crystal Engineering and Catalysis*”
- Supervisor: **Prof. Sanjay K. Mandal**

07/2010 – 06/2012 **Master of Science in Analytical Chemistry**

- Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad, India.
- Grade: First class (72.17%)
- Industrial Project: *In-Plant Training* at Orchid Chemicals & Pharma Ltd., MIDC-Waluj, Aurangabad, Maharashtra, India.

Awards, Scholarships and Academic Achievements:

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|-------------|--|
| 2013 | Qualified CSIR-UGC NET (Council of Scientific & Industrial Research-University Grants Commission-National Eligibility Test) with All India Rank 79 . |
| 2014 | Qualified GATE (Graduate Aptitude Test in Engineering) with All India Rank 132 . |
| 2014 – 2017 | Awarded Junior Research Fellowship from University Grants Commission (UGC) India. |
| 2017 – 2019 | Awarded Senior Research Fellowship from University Grants Commission (UGC) India. |
| 2015 – 2016 | Teaching Assistant at IISER Mohali:
✓ Chemistry Lab I ✓ Organic Chemistry Lab |

Research Experience and Technical Proficiencies:

➤ Research Skills and Instrument Expertise

- Organic synthesis: experienced in design and synthesis of novel multi-step organic small molecules/ ligands and peptides.
- Inorganic synthesis: expertise in designing and synthesis of multifunctional materials (Metal-organic frameworks (MOFs) and coordination polymers) under solvo/ hydro-thermal, and room temperature conditions.
- Experienced in preparation and handling of air, moisture sensitive reagents/ reactions (using Schlenk line, Glove box), and crystallization techniques.
- Trained and skilled in strategic MOFs based heterogeneous catalysts designing, catalytic organic transformations, and mechanistic investigations using advanced analytical techniques.
- Expertise in the design and building of custom GC packed columns for chemical separation.
- Expertise in single crystal data collection and refinement, structure solution, disorder modeling, weak interaction study, Hirshfeld surface analysis, topological analysis, void calculation, and presentation of data for publication.
- Guided undergraduate students extensively and mentored them in formulating their on projects.
- Instrument Expertise: Single Crystal X-Ray Diffractometer (*Bruker Kappa Apex II, Bruker D8 Venture, and Rigaku 007HF Mo rotating anode*), Powder X-ray Diffractometer (*Bruker D8 Advance, Bruker D8 Discover, and Rigaku Ultima IV*), Thermal Analysis Instruments (*TGA, DTA and DSC by Shimadzu*), Spectroscopy (NMR (*Bruker 400*), HRMS, FTIR & ATR (*Agilent*), and UV-Vis (solid and liquid state, *Agilent Cary-5000*)), GC (*Agilent*), HPLC, Fluorimeter (*Horiba*), CombiFlash, SEM, EDX, XPS, Tube Furnace, Hot Stage Microscopy.
- Software's: ChemDraw, OriginPro, APEX3, CrysAlisPro, Olex², Mercury, CrystalExplorer, Diamond, TOPAS-Academic, CSD data base, ICDD, PLATON, ToposPro, Ortep3, Viewer Lite, Biovia Discovery Studio, X'Pert HighScore Plus, CrystalMaker, PyMol, VESTA, SpinWorks, MestreNova, MS-Office, Mendeley.

List of Publications:

- 1) **Markad, D.**; Mandal, S. K. "An Exploration into the Amide–Pseudo Amide Hydrogen Bonding Synthron between a New Coformer with Two Primary Amide Groups and Theophylline"
CrystEngComm **2017**, *19*, 7112-7124. [[Selected for a back-cover page](#)]
- 2) **Markad, D.**; Mandal, S. K. "Amide–Pseudo Amide Motif in the Co-crystal of Theophylline and Bis(amide) Coformers"
Acta Crystallogr. Sect. A Found. Adv. **2017**, *73*, C664.
- 3) **Markad, D.**; Mandal, S. K. "Synthesis and Structural Characterization of a Novel Dinuclear Cu(II) Complex: an Efficient and Recyclable Bifunctional Heterogeneous Catalyst for the Diastereoselective Henry Reaction"
Dalton Trans. **2018**, *47*, 5928-5932. [[Selected for a back-cover page](#)]
- 4) **Markad, D.**; Khullar, S.; Mandal, S. K. "Engineering a Nanoscale Primary Amide Functionalized 2D Coordination Polymer as an Efficient and Recyclable Heterogeneous Catalyst for the Knoevenagel Condensation Reaction"
ACS Appl. Nano Mater. **2018**, *1*, 5226-5236.
- 5) Mahesha, C. K.; Agarwal, D. S.; Karishma, P.; **Markad, D.**; Mandal, S. K.; Sakhuja, R. "Iridium-catalyzed [4 + 2] Annulation of 1-arylidazolones with α -diazo carbonyl Compounds: Access to Indazolone-fused Cinnolines"
Org. Biomol. Chem. **2018**, *16*, 8585-8595.

- 6) Kumari, S.; Shakoore, S. M. A.; **Markad, D.**; Mandal S. K.; Sakhuja, R. "NH₄OAc-promoted Cascade Approach towards Aberrant Synthesis of Chromene-fused Quinolinones"
Eur. J. Org. Chem. **2019**, *4*, 705-714.
- 7) **Markad, D.**; Khullar, S.; Mandal, S. K. "Novel Primary Amide-based Cationic Metal Complexes: Green Synthesis, Crystal Structures, Hirshfeld Surface Analysis and Solvent-free Cyanosilylation Reaction"
Dalton Trans. **2019**, *48*, 3743-3757.
- 8) **Markad, D.**; Mandal, S. K. "Design of a Primary Amide-Functionalized Highly Efficient and Recyclable Hydrogen-Bond-Donating Heterogeneous Catalyst for the Friedel-Crafts Alkylation of Indoles with β - Nitrostyrenes"
ACS Catal. **2019**, *9*, 3165-3173.
- 9) Tayade, S. B.; Lllathvalappil, R.; Lapalikar, V.; **Markad, D.**; Kurungot, S.; Pujari, B.; Kumbhar, A. S. "Copper(II)-coordination Polymer Based on a Sulfonic-Carboxylic Ligand Exhibits High Water-facilitated Proton Conductivity"
Dalton Trans. **2019**, *48*, 11034-11044.
- 10) Tayade, S. B.; **Markad, D.**; Kumbhar, A. S.; Erxleben, A.; Chakravarty, D. "Coordination Polymers of Cd II and Pb II Derived from Bipyridine–Glycoluril: Influence of Metal-Ion Size"
Acta Crystallogr. Sect. C Struct. Chem. **2019**, *75*, 1084-1090.
- 11) **Markad, D.**; Khullar, S.; Mandal, S. K. "Design and Development of a Heterogeneous Catalyst for the Michael Addition of Malononitrile to 2-Enoylpyridines: Influence of the Primary Amide Decorated Framework on Catalytic Activity and Selectivity"
Inorg. Chem. **2019**, *58*, 12547-12554.
- 12) Haneef, J.; **Markad, D.**; Chadha, R. "Interaction Maps Driven Cococrystallization of Ambrisentan: Structural and Biopharmaceutical Evaluation"
Cryst. Growth Des. **2020**, *20*, 4612-4620.
- 13) Ubale, P. A.; Kollur, S. P.; Bansode P. A.; Chavan, S.; Karhale S. S.; Nishad, A.; Helavi, V. B.; **Markad, D.**; Castro, J. O.; Frau, J.; et al. "In Vitro Anticancer Activity of 4(3H)-Quinazolinone Derived Schiff base and its Cu(II), Zn(II) and Cd(II) Complexes: Preparation, X-ray Structural, Spectral Characterization and Theoretical Investigations"
Inorganica Chim. Acta **2020**, *511*, 119846.
- 14) **Markad, D.**; Khullar, S.; Mandal, S. K. "A Primary Amide-Functionalized Heterogeneous Catalyst for the Synthesis of Coumarin-3-carboxylic Acids via a Tandem Reaction"
Inorg. Chem. **2020**, *59*, 11407-11416.
- 15) Baig, F.; Jaswal, V.; Rangan, K.; Khullar, S.; **Markad, D.**; Sarkar, M. "Positional Effects of a Pyridyl Group in Zn(II) Coordination Polymers on the Selective Dye Adsorption Properties"
Polyhedron **2022**, *214*, 115646.
- 16) Das, M.; **Markad, D.**; Maity, S.; Ghosh, P.; Sarkar, M. "Bis(pyridyl)-disulfonamides: Structural Comparison with their Carboxamidic Analogues and the Effect of Molecular Geometry and Supramolecular Assembly on their Photophysical Properties"
New J. Chem. **2022**, *46*, 7374-7384.
- 17) Laha, B.; Khullar, S.; **Markad, D.**; Mandal, S. K. "Room Temperature Synthesis of New Isorecticular 2D Metal–organic Frameworks of Co(II) and Ni(II) Comprised of Dual Semiflexible Neutral and Anionic Linkers, and Their Conversion to Metal Oxide Nanomaterials"
Inorganica Chim. Acta **2022**, *539*, 120966.
- 18) Khullar, S.; Janak; Sakshi; Saini, H.; Sapner, V. S.; Sathe, B. R.; **Markad, D.** "Design and Synthesis of Lead(II)-Based Electrocatalysts for Oxygen Evolution Reaction"
Inorg. Chem. **2022**, *61*, 7579-7589.

19) Arora, Z.; **Markad, D.**; Khullar, S.; Mondal, S.; Mandal, S. K. “Enhanced Catalytic Activity of a Cd(II) Complex Containing an Unsymmetrical Primary Amide Functionalized Ligand for the Solvent-Free Cyanosilylation Reaction”

Catal Lett **2023**, *153*, 2036-2044.

20) Khan, S.; **Markad, D.**; Mandal, S. K. “Two Zn(II)/Cd(II) Coordination Polymers as Recyclable Heterogeneous Catalysts for an Efficient Room-Temperature Synthesis of α -Aminonitriles *via* the Solvent-Free Strecker Reaction”

Inorg. Chem. **2023**, *62*, 275–284.

21) Haneef, J.; **Markad, D.**; Chadha, R.; Kumar, A.; Kumar N. “Structural insights into mechanical anisotropy in ambrisentan polymorphs”

CrystEngComm **2023**.

Conferences/ Symposia:

- Participated in the 13th Eurasia conference on chemical science, held at Indian institute of science, Bangalore, India, (14-18 Dec, 2014).
- Poster presentation entitled “Novel Bifunctional Metal Organic Coordination Networks for Catalysis” at the Inter-IISER Chemistry Meet 2017 (IICM 2017), and received **Best Poster award** held at Indian Institute of Science Education and Research (IISER), Bhopal, India (20-22 Jan, 2017).
- Poster presentation entitled “Amide-pseudoamide motif in the co-crystal of Theophylline and bis(amide) cofomers” at 24th Congress and General Assembly of the International Union of Crystallography (IUCr), held at Hyderabad, India (21-28 Aug, 2017) and certified. [Article Link](#)
- Poster presentation entitled “Primary Amide Sidearm in Metal-Organic Framework as Catalytically Active Hydrogen-Bond Heterogeneous Catalyst for Michael Addition of Malononitrile to 2-Enoylpyridines” at the International symposium on Modern Trends in Inorganic Chemistry-XVII (MTIC-XVII), held at NCL Pune, India (11-14 Dec, 2017) and certified.

References:

- **Prof. Matthew Rosseinsky FRS** (Postdoctoral adviser)
Professor at Department of Chemistry,
University of Liverpool, United Kingdom.
E-mail: m.j.rosseinsky@liverpool.ac.uk
- **Prof. Sanjay K. Mandal** (Ph. D. supervisor)
Professor at Department of Chemical Sciences,
Indian Institute of Science Education and Research (IISER) Mohali, India.
E-mail: sanjaymandal@iisermohali.ac.in
- **Dr. Sadhika Khullar**
Assistant Professor at Department of Chemistry,
Dr. B. R. Ambedkar National Institute of Technology (NIT), Jalandhar, India.
E-mail: khullars@nitj.ac.in

Personal Information:

Date of birth: January 1, 1990

Gender: Male

Citizenship: Indian

Marital status: Married

Declaration:

I hereby declare that the above statements and information are correct to the best of my knowledge and belief.

DATTA MARKAD