Name: Dr. M. Jaya Prakash Designation: Assistant Professor Address: Room No: MC-314

Department of Chemistry,

N.I.T., Rourkela, Odisha – 769 008.

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Academic Profile:

• M. Sc. : (General Chemistry), School of Chemistry, University of Hyderabad, India.

• Ph. D.: (Materials Chemistry), School of Chemistry, University of Hyderabad, India.

Academic Distinctions:

- CSIR-JRF (2002-2004)
- CSIR-SRF
- Young Scientist Research Award (2007) from Dr. K. V. Rao Scientific Society.

Research and Professional Experience:

- Assistant Professor, N.I.T, Rourkela, India: February 2014 onwards.
- Postdoctoral Research Fellow, Department of Chemistry & Biochemistry, University of Notre Dame, U.S.A.: October 2010 May 2012.
- Postdoctoral Research Fellow, Department of Applied Chemistry, Hanyang University at Ansan, South Korea.: July 2008 September 2010.

Research Interests:

Materials Chemistry: Synthesis and studying the various applications of functional materials.

- 1. Porous covalent organic cage molecules for Carbon dioxide gas adsorption applications.
- 2. Fluorescent porous cage molecules for analytical chemical applications.
- 3. Novel drug molecules for anti-cancer applications.
- 4. Porous metal-organic polyhedral molecules for guest molecule encapsulation and catalytic applications.
- 5. Graphite oxide materials for potential gas adsorption applications.

Computational Chemistry: Modeling and estimation of various physical quantities of molecules and molecular clusters by semi-empirical and ab initio methods.

1. Estimation of various thermodynamic quantities and stability of molecules and materials by semi-empirical methods included in software like MOPAC.

2. Ab initio and DFT computational methods built-in GAUSSIAN for studying the stability and various optical properties of molecules and materials.

Publications:

From NIT Rourkela:

1. Pilli Govindaiah, Sushant Kumar Jena, Sabhavat Krishna, Rupak Kishor, M. Jaya Prakash

Carbon dioxide gas adsorption in Mesoporous Covalent organic Imine polymers: Influence of terminal amine functional groups on gas adsorption. (https://doi.org/10.26434/chemrxiv.5826435.v1.)

2. Pilli Govindaiah, Naresh Dumala, Paramjit Grover, M. Jaya Prakash.

Synthesis and biological evaluation of novel 4,7-dihydroxycoumarin derivatives as anticancer agents.

Organic & Medicinal Chemistry Letters 2019, 29, 1819 - 1824.

3. Pilli Govindaiah, Irshad Mattan, Naresh Dumala, M. Jaya Prakash, Paramjit Grover.

Design, Synthesis, Biological and *In silico* evaluation of Coumarin-hydrazone Derivatives as Tubulin targeted Antiproliferative agents.

Bioorganic Chemistry **2019**, 91, 103143.

4. Govindaiah Pilli, Naresh Dumala, Jamuna S. Sreeja, Rince John, Suparna Sengupta, Paramjit Grover, M. Jaya Prakash

Design, Synthesis and Pharmacological Evaluation of 4-Hydroxycoumarin Derivatives as Antiproliferative Agents.

ChemistrySelect **2019**, *4*, 10805 – 10809.

5. Ramesh Kumar Gajula, Rupak Kishor, and M. Jaya Prakash

Imine-Linked Covalent Organic Cage Porous Crystals for CO₂ Adsorption.

ChemistrySelect **2019**, 4, 12547–12555.

From post-doctoral work period:

1. M. Java Prakash, Allen G. Oliver, and Slavi C. Sevov *Cryst. Growth Des.*, 2012, 12, 2684–2690

Guest-Host Frameworks of the Anionic Metal Complex $[Fe(ox)_3]^3$ and Cationic Bipyridinium-Based Linkers Bonded by Charge-Assisted Hydrogen Bonds.

2. M. Jaya Prakash, Slavi C. Sevov, *Inorg. Chem.*, 2011, 50, 12739-12746.

Hydrogen-Bonded Inclusion Compounds with Reversed Polarity: Anionic Metal-Complexes and Cationic Organic Linkers.

3. <u>M. Jaya Prakash</u>, Minhak Oh, Xinfang Liu, Kwi Nam Han, Gi Hun Seong, Myoung Soo Lah, *Chem. Commun.*, **2010**, *46*, 2049 – 2051.

Edge-directed $[(M_2)_2L_4]$ tetragonal metal-organic polyhedra decorated using a square paddle-wheel secondary building unit.

4. **M. Jaya Prakash**, Myoung Soo Lah, *Chem. Commun.*, **2009**, *45*, 3326 – 3341.

Metal-organic macrocycles, metal-organic polyhedral and metal-organic frameworks. (Feature Article).

5. <u>M. Jaya Prakash</u>, Yang Zou, Seunghee Hong, Mira Park, Minh-Phuong Ngoc Bui, Gi Hun Seong, Myoung Soo Lah, *Inorg. Chem.*, **2009**, *48*, 1281 – 1283.

Metal-Organic Polyhedron Based on a Cu(II) Paddle-Wheel Secondary Building Unit at the Truncated Octahedron Corners.

From Ph. D. period:

1. M. Jaya Prakash, P. Raghavaiah, Y. S. R. Krishna, T. P. Radhakrishnan, *Angew. Chem., Int. Ed.*, 2008, 47, 3969 – 3972.

Growing molecular crystal on inorganic crystal surface: polar structure induced by noncentrosymmetric template.

2. S. Philip Anthony, M. Java Prakash, T. P. Radhakrishnan, Mol. Cryst. Liq. Cryst., 2007, 473, 67 – 85.

*C*₂-symmetric Bis(amide) Molecules : Solid State Assembly, Thermal Stability and Second Harmonic Generation.

3. **M. Java Prakash**, T. P. Radhakrishnan, *Inorg. Chem.*, **2006**, *45*, 9758 - 9764.

SHG Active Crystals of a Remote Functionalized Achiral NLO-phore Assembled through Zinc(II) Complexation.

4. M. Jaya Prakash, T. P. Radhakrishnan, Chem. Mater., 2006, 18, 2943 - 2949.

Second Harmonic Generation from a Homologous Series of Molecular Crystals: Impact of Supramolecular Interactions.

5. M. Java Prakash, T. P. Radhakrishnan, Cryst. Growth Des., 2005, 5, 1831-1836.

Remote Functionalized Nonlinear Optical Chromophore: Optimal Assembly in Crystals for Second Harmonic Generation.

6. **M. Jaya Prakash**, T. P. Radhakrishnan, *Cryst. Growth Des.*, **2005**, *5*, 721-725.

SHG Active Salts of 4-Nitrophenolate with H-Bonded Helical Formations: Structure-Directing Role of ortho-Aminopyridines.

Sponsored Research Projects

SI. No.	Title of the project	Funding agency	Total Financial outlay	Year of start & total period	Names of P.I. and other investigators	Status (completed, in progress or proposal submitted)
1.	Nitrogen rich Covalent Organic Cage molecule based materials for Carbon Dioxide Capture applications	DST- SERB- ECRA	₹ 28,00,000/-	March 2016, 3 years.	Dr. M. Jaya Prakash	In Progress.
2.	Covalent Organic Polymers based materials for carbon dioxide gas adsorption applications.	TEQIP-II.	₹ 1,50,000/-	September, 2016. One year.	Dr. M. Jaya Prakash	Completed.

Poster / Lecture Presentations in conferences:

- 1. Poster presented at the Fourth DAE-BRNS National Laser Symposium (NLS 4) at BARC, Mumbai, 10 13 January, 2005.
 - M. Java Prakash, D. Narayana Rao, T. P. Radhakrishnan

Helical Organization and Optimal Orientation of NLO-phores in Novel Molecular Crystals for Second Harmonic Generation

- 2. Poster presented at the 8th international conference on optoelectronics, Fiber optics & Photonics, Hyderabad, India, December 13 16, 2006.
 - M. Jaya Prakash, T. P. Radhakrishnan

Novel Molecular Crystals and Metal Complexes for Second Harmonic Generation Developed through the Remote Functional Group Approach

3. Poster presented in JSPS-DST Asia Academic Seminar on Molecular and Supramolecular Materials with Designed Functions, February 23-28, 2007, Pune, India.

M. Java Prakash, T. P. Radhakrishnan

Materials for Optical Second Harmonic Generation Based on Remote Functionalized Molecules.

4. Lecture presented at Dr. K. V. Rao 7th Annual Young Scientist Award competition, Hyderabad, April 2007.

M. Jaya Prakash

Remote Functionality and Templating Chiral Surfaces for Noncentrosymmetric Crystal Lattice Formation for SHG Application.

5. Lecture presented at 4th annual in-house symposium CHEMFEST-07, march 2007.

M. Jaya Prakash

Remote functional molecular crystals: Enhancement of SHG property by H-bonding interactions.

- 6. Poster presented in 104th Korean Chemical Society Meeting at Daejeon, October 28-30, 2009.
 - M. Jaya Prakash, Minhak Oh, Xinfang Liu, Myoung Soo Lah

Metal-Organic Polyhedra Decorated Using a Square Paddle-wheel Secondary Building Unit.

Workshops and training classes attended:

- 1. SERC Summer School on "Solid State and Materials Chemistry", SSCU, Indian Institute of Science, Bangalore, July 2005.
- 2. Bruker-AXS single crystal X-ray diffractometer User's workshop, May 30 June 1, 2006.