

## Dr. Devendra Singh

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**Date of Birth:** 01-07-1984

**Sex:** Male

**Marital status:** Married

## Education

- 2007-2012: **PhD in Chemistry**, Title of thesis "Supramolecular chemistry of cyclic imides tethered carboxylic acids and related compounds" **April 2012**, Indian Institute of Technology Guwahati, India.
- 2003-2005: **Master of Science (Chemistry), first class**, Dr. B. R. A. University, Agra, India.
- 2000-2003: **Bachelor of Science (Chemistry), first class**, University of Rajasthan, Jaipur, India.

## Honors and Awards

- Qualified the **Graduate Aptitude Test for Engineering (GATE)** 2007: Percentile score 97.69 (All India Rank 108).
- Qualified the Joint **CSIR-UGC Test for Junior Research Fellowship and Eligibility for Lectureship (NET)** in 2007, held by the Council of Scientific and Industrial Research (CSIR).
- Upgraded to **CSIR-Senior Research Fellowship (CSIR-SRF)** in 2010.

## Experiences

- **June 2018-Present:** Assistant Professor, Department of Chemistry, Mohan Lal Sukhadia University Udaipur, Rajasthan, India.
- **August 2015-June 2018:** Assistant Professor, Department of Chemistry, PDM University Bahadurgarh, Haryana, India.
- **July 2012-July 2015:** **Post-doctoral Research Associate**, Pohang University of Science & Technology, Republic of Korea and Kyoto University Japan, respectively.
- **2010-12:** **Senior Research Fellow** in Department of Chemistry, Indian Institute of Technology Guwahati, from the Council for Scientific and Industrial Research (CSIR), India.
- **2007-09:** **Junior Research Fellow** in Department of Chemistry, Indian Institute of Technology Guwahati, from the Council for Scientific and Industrial Research (CSIR), India.

## Research Interest

Supramolecular Chemistry is of current interest due to its applications in catalysis, separation techniques and as potential storage materials. My research approaches this area by particularly emphasizing on:

- Host-guest self assembled networks, low molecular mass organic gelators (LMOG), multicomponent cocrystals of active pharmaceutical ingredients.
- Macrocyclic systems as potential building blocks for ion and molecular recognition, fluorescent and colorimetric chemosensors etc.
- Porous crystalline covalent organic frameworks for gas storage and catalytic applications.
- Organic-inorganic hybrid materials and metal-organic frameworks for selective gas sorption.
- Catalysis and electrochemical studies of redox-active metal-organic materials.
- Magnetic, electric and optical properties of nitroxide radical liquid crystalline materials.

## Research Publications

1. **Devendra Singh**, Katsuaki Suzuki, Koji Taguchi, Rui Tamura. Magneto-LC effects in supramolecular organic chiral nitroxide biradical liquid crystalline materials based on paramagnetic pyrrolidine core. (manuscript in preparation)
2. **Devendra Singh**, Dongwook Kim, Myoung S. Lah, Kwang S. Kim. Design and construction of multifunctional porous organic fluorescent supramolecular architectures. (manuscript in preparation).
3. K. Singh, A. K. Singh, **Devendra Singh**, R. Singh, Siddharth Sharma. Pd/Fe<sub>3</sub>O<sub>4</sub> supported on nitrogen-doped reduced graphene oxide for room-temperature isocyanide insertion reactions. *Catal. Sci. Technol.*, **2016**, 6, 3723-3726 (IF: 5.773).
4. Siddharth Sharma, Ajay K. Singh, **Devendra Singh** and Dong-Pyo Kim. Chemical Fixation of Carbon Dioxide by Copper (II) Catalyzed Multicomponent Reactions for Oxazolidinedione Syntheses. *Green Chem.*, **2015**, 17, 1404-1407. (IF 9.125).
5. Dongwook Kim, Xinfang Liu, Minhak Oh, Xiaokai Song, Yang Zou, **Devendra Singh**, Kwang S. Kim, Myoung S. Lah. Isoreticular metal-organic frameworks based on a rhombic dodecahedral metal-organic polyhedron as a tertiary building unit. *CrystEngComm.*, **2014**, 16, 6391-6397. (IF 4.034).
6. **Devendra Singh**, Jubaraj B. Baruah. Hydrocarboxylates of manganese, copper and zinc. *Inorg. Chim. Acta*, **2013**, 394, 703-709. (IF 2.046).

7. **Devendra Singh**, Jubaraj B. Baruah. Guest inclusion in cyclic imides connected to carboxylic acid by flexible tether. *J Incl Phenom Macrocycl Chem.*, **2013**, *76*, 269-81. (IF 1.488).
8. **Devendra Singh**, Jubaraj B. Baruah. Solid state assemblies of cyclic imides tethered hydroxy benzoic acids with pyridine and quinoline: toward the formation of channels and cavities. *Cryst. Growth Des.* **2012**, *12*, 3169-3180. (IF 4.891).
9. **Devendra Singh**, Jubaraj B. Baruah. Metal (II) complexes derived from conformation flexible cyclic imides tethered carboxylic acids: syntheses, supramolecular structures, and molecular properties. *Cryst. Growth Des.* **2012**, *12*, 2109-2121. (IF 4.891).
10. **Devendra Singh**, Jubaraj B. Baruah. Molecular complex from two different binuclear copper 1,4,5,8-naphthalenetetracarboxylate complexes. *Inorg. Chim. Acta*, **2012**, *390*, 37-40. (IF 2.046).
11. **Devendra Singh**, Jubaraj B. Baruah. Structural study on solvates of dopamine-based cyclic imide derivatives. *Cryst. Growth Des.* **2011**, *11*, 768-777. (IF 4.891).
12. **Devendra Singh**, Pradeep Bhattacharyya, Jubaraj B. Baruah. Structural studies on solvates of cyclic imide tethered carboxylic acids with pyridine and quinoline. *Cryst. Growth Des.* **2010**, *10*, 348-356. (IF 4.891).
13. **Devendra Singh**, Subrata K. Ghosh, Jubaraj B. Baruah. Solvent-dependent fluorescence emission in heterocyclic compounds having isoquinoline backbone. *J. Heterocycl. Chem.* **2010**, *47*, 199-206. (IF 0.893).
14. **Devendra Singh**, Jubaraj B. Baruah. Varieties in symmetry non-equivalent structural arrangements in solvates of 2-(3-methylene-1,3,7-trioxo-6-(2-carboxy-phenyl)-3,5,6,7-tetrahydro-1H-pyrrolo[3,4f]isoindol-2-yl)benzoic acid. *J. Mol. Struct.*, **2009**, *937*, 75-80. (IF 1.753).
15. **Devendra Singh**, Jubaraj B. Baruah. Different solvates of two isomeric dicarboxylic acids with pyridine and quinoline. *CrystEngComm.*, **2009**, *11*, 2688-2694. (IF 4.034).
16. **Devendra Singh**, Jubaraj B. Baruah. Solvation controlling reaction paths and gel-formation in imide derivatives. *Tet. Letters*, **2008**, *49*, 4374-4377. (IF 2.379).

## Outline of Postdoctoral Work from Kyoto University

During my post-doctoral research at Kyoto University, I have been focused on synthesis and studies of magnetic, electrical and optical properties of All-organic, Metal-organic and Supramolecular-organic nitroxide biradical liquid crystalline (LC) materials those are paramagnetic and have potential applications in the field of optical data storage devices, biomedical and semiconductors.

In this context, using multistep synthetic procedures, we have synthesized chiral all-organic (**A**), Metal-organic (**B**) and Supramolecular-organic (**C**) nitroxide biradical LC compounds (Fig 1), which contain

polar and chiral cyclic-nitroxide units in the mesogen core, are thermally stable up to 150 °C in the air and can show LC phases over a wide temperature range below 90 °C. Magnetic, electrical and optical properties of these nitroxide biradical LC materials are under investigation.

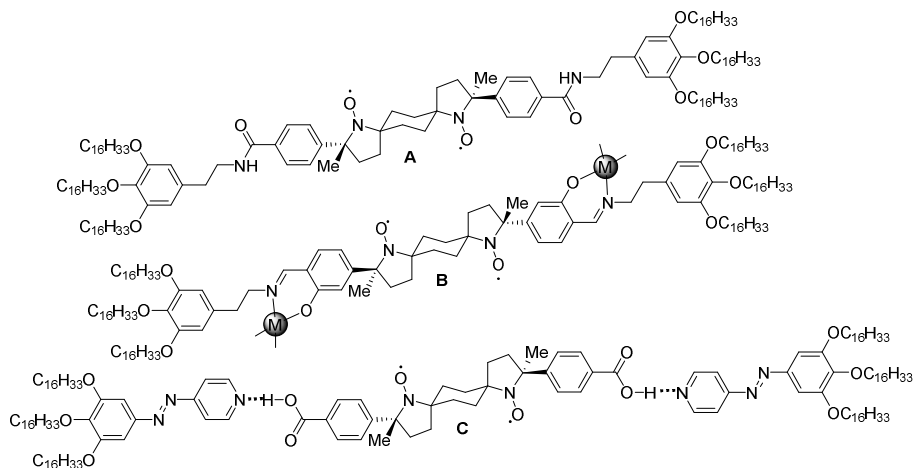


Fig 1: All-organic (A), Metal-organic (B), Supramolecular-organic (C) nitroxide biradical LC materials.

## Outline of Postdoctoral Work from POSTECH

During my postdoctoral research at the Pohang University of Science & Technology, I have been directed toward the design and synthesis of new multifunctional organic molecules for various supramolecular aspects such as organic gelation, anion and cation binding studies, host-guest inclusion chemistry and metal-organic frameworks. Based on these considerations, several multifunctional molecules (some of them are shown Fig 2) have been synthesized. The physical properties of the gels formed by compound **A** and **B** along with their spectroscopic, microscopic and rheological properties are studied. Single crystal X-ray structure of gelator molecules with anion and theoretical calculations on possible weak interactions which are responsible for gel formation are investigated. The compounds **C** and **D** as well as some other isomeric compounds have been used as host to prepare supramolecular-organic frameworks (SOF) with some newly synthesized N-containing (bis-imidazole, bis-pyridine, bis-quinoline) guests. Subtle differences in hydrogen bonding patterns lead to diverse architectures in a series of isomeric supramolecular fluorescent materials.

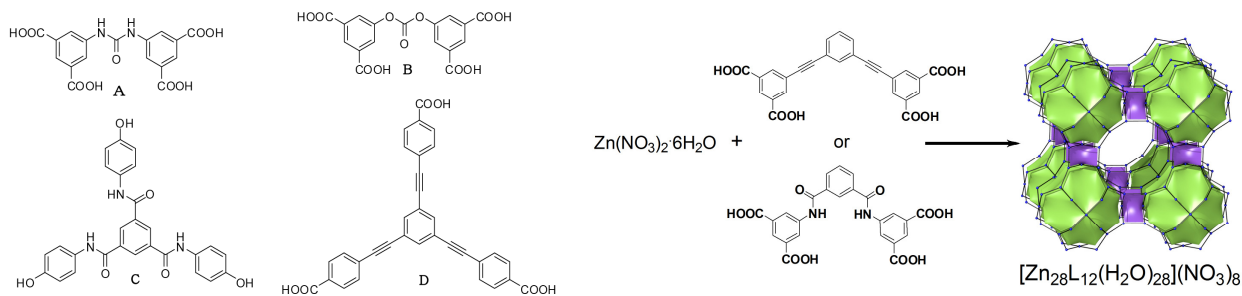


Fig 2. Structures of some host compounds along with their MOF unit.

Moreover, the efforts have also been made toward the production of metal-organic frameworks (MOFs) of some multicarboxylate ligands with exciting applications in gas adsorption and catalysis. The solvothermal reactions of Zn(II) ion with ligands containing two 1,3-benzene dicarboxylate residues resulted in isorecticular MOFs with a 3,3,4-c **zjz** topology based on a rhombic dodecahedral metal-organic polyhedron (MOP), in which the rhombic dodecahedral MOP was built using six  $[\text{Zn}_2(\text{COO})_4]$  clusters as a 4-c SBU and eight  $[\text{Zn}_2(\text{COO})_3]$  clusters as a 3-c SBU (Fig 2).

## Outline of PhD work from IITG

During my doctoral studies, I have worked in the field of supramolecular organic and inorganic chemistry. My Ph.D. thesis entitled “*Supramolecular chemistry of cyclic imides tethered carboxylic acids and related compounds*” where I have applied bottom-up approach to synthesize various cyclic imide derivatives and studied a variety of aspects of imide chemistry including polymorphism, host-guest self-assembled networks, molecular recognition, organic gelation, solvatochromism and metal-organic frameworks. A fair amount of work is devoted to understand the role of non-covalent interactions to derive the self-assembly of complex structures. The major research accomplishments during my doctoral study are as follows:

1. Host-guest complexes of pyridine and quinoline with some of the naphthalimide or naphthalene diimide tethered aromatic hydroxy carboxylic acids are reported to create channels in their 3D supramolecular architectures (Fig 3). Formation of different types of hydrogen bonds motifs in these complexes is established by DFT calculations which suggest that their formation is controlled by the other weak interactions present in the crystal lattices (*Cryst. Growth Des.* **2010**, *10*, 348-356, *Cryst. Growth Des.* **2012**, *12*, 3169-3180).
2. Minor differences in host-guest interactions are found to be responsible for the formation of polymorphs of pyridine and quinoline solvates of naphthalene diimide and pyromellitic diimide tethered carboxylic acids (*CrystEngComm.*, **2009**, *11*, 2688-2694, *J. Mol. Struct.*, **2009**, *937*, 75-80). This generates a new kind of host-guest assemblies from amine interactions with a central dicarboxylic acid molecule to encapsulate guest amine/s. The preferential binding of quinoline over pyridine by the host is observed in the formation of polymorphic solvates which is the guiding factor for separation techniques.
3. It is realized that the symmetry non-equivalent solvates with same  $Z'$  value can have different orientations of the parent molecules depending on the solvent attached to it (*J Incl Phenom Macrocycl Chem.*, **2013**, *76*, 269-81, *Cryst. Growth Des.* submitted). The crystal packing requirement decides such orientations and leads to new kind of unusual polymorphs.

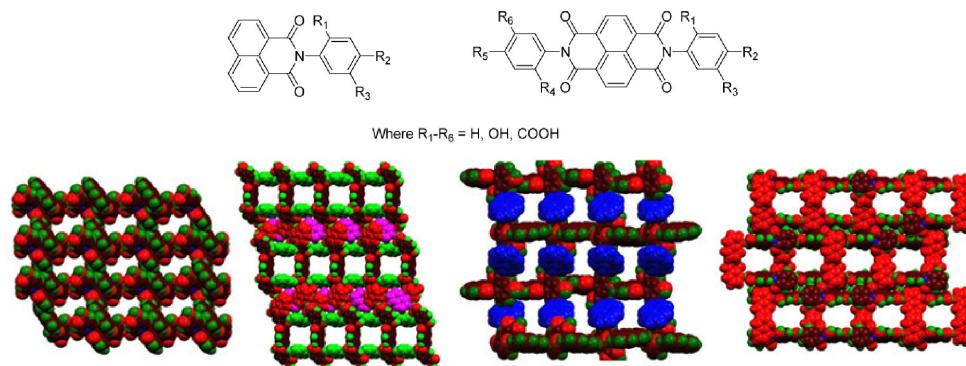


Fig 3. 3D supramolecular architectures of some of the multifunctional naphthalene diimide hosts.

4. A series of new class of low molecular weight cyclic imide organogelators is prepared and their gel formation properties are studied. The solvato-emissive properties of heterocyclic compounds derived from planar aromatic ring are also described (*Tet. Letters*, **2008**, *49*, 4374-4377, *J. Heterocycl. Chem.*, **2010**, *47*, 199-206). Different organic solvents such as dichloromethane, acetonitrile, methanol can be distinguished from the different emission wavelengths of the heterocyclic compounds.
5. A series of M(II) carboxylates of flexible hydrophobic unit coupled with cyclic imide units are prepared and their supramolecular structural features are described. It is observed that coordination environments around the metal centers as well as weak non covalent forces affect the dimensionality and features of supramolecular architectures of such metal complexes (*Cryst. Growth Des.* **2012**, *12*, 2109-2121, *Inorg. Chim. Acta*, **2013**, *394*, 703-709). Thermal studies have shown the differences of coordinated or lattice solvent molecules in these complexes. The solid state photoluminescence properties of as synthesized M(II) complexes as well as their parent ligands are also investigated.
6. Beside that, Structural study on dopamine-based imide derivatives and their solvates has also been carried out as they may have biological applications as a neurotransmitter and as drugs for several diseases (*Cryst. Growth Des.* **2011**, *11*, 768-777). Different types of metal complexes of some other multi-carboxylic acids are synthesized and some of their properties are studied during my doctoral studies (*Inorg. Chim. Acta*, **2012**, *390*, 37-40).

## Main Skills

### Scientific skills:

- Experienced towards organic and inorganic syntheses, protective atmosphere synthesis (air free synthetic techniques using schlenk line, glove box), hydro/solvothermal synthesis.

- Experience of synthesizing liquid crystalline materials, ionic liquids and uses of various crystallization techniques for inorganic and organic complexes.
- Have experience of working with FT-IR spectrometer, UV-Vis-NIR spectrometer and fluorimeter to study samples at solid and liquid state.
- Have been used HPLC, NMR, Mass (LC-MS, GC-MS), ESR spectrometer.
- Have also been used electrochemical analyzer, gas adsorption analyzer, magnetic susceptibility balance, TGA, DSC, SEM, TEM and PXRD.
- Have extensive experience of using single crystal X-ray diffractometer (Bruker Nonius Smart Apex 2 and Rigaku Rapid Auto) along with complete data processing.
- Have experience of carrying out theoretical calculations such as structure optimization, time dependent DFT calculations using Gaussian 03W software.

#### **Computer skills:**

- Operating Systems: Windows.
- Softwares Familiar with: MS-Office, Adobe illustrator, Adobe Photoshop, ChemOffice, ISIS draw, Sigma plot, Nuts, Delta, Origin, Gaussian 03W, Mercury, ORTEP, Diamond 3, Rasmol, WinGX, SHELX-97, APEX2.

#### **Extra skills:**

- Writing and preparing manuscripts, participating in team efforts, guiding graduate and undergraduate students,
- Independent thinking, excellent oral, communication and presentation skills.

### Seminars and Workshop

- 12th International Symposium on Inorganic Ring Systems (IRIS 12), August 2009, held at Holiday Inn Resort Goa, Organized by the Department of Chemistry, Indian Institute of Technology Bombay.
- DAE-BRNS 3rd International Symposium on Materials Chemistry (ISMC-2010), December 2010, (**Best Poster Award**) held at Bhabha Atomic Research Centre, Mumbai.
- 13th CRSI National Symposium in Chemistry and 5th CRSI-RSC Symposium in Chemistry, February 2011, held at National Institute of Science Education and Research (NISER), Bhubaneswar.
- 4<sup>th</sup> Asian Conference on Coordination Chemistry (ACCC4), November 2013, held at International Convention Center, Jeju, Republic of Korea.