



# INDO-FRENCH LABORATORY OF SOLID-STATE CHEMISTRY WORKSHOP- 2022

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SSCU Auditorium 03-04 October, 2022

# BOOK OF ABSTRACTS

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#### Schedule of the LAFICS Workshop 03<sup>rd</sup> -04<sup>th</sup> October 2022

Time	Monday 03-10-2022	Time	Tuesday 04-10-2022
Session I	Session Chair: Session Chair 1	Session IV	Session Chair: Session Chair 4
09:30 – 09:40	Inaugural Session	09:00- 09:30	Valerie Pralong
09:40- 10:00	Dr. Srini Kaveri 🛛 🤟	09:30 – 10:00	Awadhesh Narayan
10:00 – 10:30	Jean Francois Dayen	10:00 – 10:30	Phani Kumar
10:30 – 11:00	Coffee Break and Poster Session	10:30 – 11:00	Coffee Break and Poster Session
Session II	Session Chair: Session Chair 2	Session V	Session Chair: Session Chair 5
11:00 – 11:30	Kanishka Biswas	11:00 – 11:30	Marie Guignard
11:30 – 12:00	Cyril Aymonier	11:30 – 12:00	A. Sundaresan
12:0 <mark>0</mark> – 12:30	Umesh V. Waghmare	12:00 – 12:30	Sheetal Kumar Jain
12:30 – 12:45	Shashwat Singh	12:30 – 12:45	Krishna Kaushik
12:45-13:00	Neha Chauhan	12.45 - 14.00	Lunch and Poster Session
13:00 – 14:00	Lunch and Poster Session	12.45 14.00	
Session III	Session Chair: Session Chair 3	Session VI	Session Chair: Session Chair 6
14:00 – 14:30	Subhash Thota	14:00 – 14:30	Naga Phani Aetukuri
14:30– 15:00	Pierre Rabu	14:30 – 15:00	Sebastian Peter
15:00–15:30	Vivek Tiwari	15:00 – 15:30	Ravishankar Narayan
15:30– 16:00	Prahallad Padhan	15:30– 15:45	Sunil Kumar
16:00– 16:15	Subham Kumar Saha	15:45 –16:00	Cyril Aymonier
16:15 –17:00	Coffee Break and Poster Session	16:00–16:30	Concluding Session
19:00	Dinner at Main Guest House Lawn	16:30	Lab Tour and Interaction

## PROGRAM

#### Monday, 03rd October 2022

#### Session – I Session Chair: Session Chair 1

09:30-09:40 Inaugural Session Welcome by Satish Patil, Chair SSCU and Marie-Helen Delville, ICMCB,

#### **CNRS Bordeaux**

09:40-10:00 *Srini Kaveri,* CNRS Paris Collaborations with France and CNRS: Opportunities and Mechanisms

10:00–10:30 *Jean Francois Dayen*, IPCMS Strasbourg Mixed Dimensional Heterostructures: a promising platform to explore innovative Advanced Materials and Devices

10:30-11:00 Coffee Break and Poster Session at SSCU Foyer

Session – II Session Chair: Session Chair 2

11:00-11:30 *Kanishka Biswas,* JNCASR Bangalore Glass-like Thermal Conductivity in a Single Crystal of Layered Metal Halides

11:30-12:00 *Cyril Aymonier,* ICMCB Bordeaux Circular chemistry in supercritical fluids for advanced functional materials

12:00-12:30 Umesh V. Waghmare, JNCASR Bangalore Metavalent Bonding Origins of Unusual Properties of Group IV Chalcogenides

12:30-12:45 **Shashwat Singh,** IISc Bangalore Hydroxysulfates as cathode materials for rechargeable batteries

12:45-13:00 Neha Chauhan, IISc Bangalore Near-IR organic photodetector

13:00-14:00 Lunch and Poster Session at SSCU Foyer

#### Session – III Session Chair: Session Chair 3

14:00–14:30 Subhash Thota, IIT, Guwahati

Unraveling the Novel Magnetic Properties of Columbites: An Emphasis on the Tricritical Point in H-T Phase diagram

14:30–15:00 *Pierre Rabu,* IPCMS, Strasbourg Multifunctional hybrid layered materials: synthesis and structure - property relationships

15:00-15:30 Vivek Tiwari, IISc Bangalore Multidimensional Electronic Spectroscopy with Combined Spectral, Temporal, and Spatial Resolution

15:30–16:00 **Prahallad Padhan,** IIT Madras Magnetocaloric Effect in (111) Oriented La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> – SrRuO<sub>3</sub> Superlattices

16:00-16:15 **Subham Kumar Saha**, IISc Bangalore Microscopy of Engineered High Interface Area Nanostructures

16:15-17:00 Coffee Break and Poster Session at SSCU Foyer

19:00 Dinner at Main Guest House lawn

#### TUESDAY, 04TH OCTOBER 2022

#### Session -IV: Session Chair: Session Chair 4

09:00-09:30 *Valerie Pralong,* CRISMAT, Caen Design of new ionic conductor used as electrode or solid electrolyte for non-aqueous batteries

09:30-10:00 *Awadhesh Narayan,* IISc Bangalore Berry curvature dipole in two-dimensional materials

10:00-10:30 *Phani Kumar,* IIT Madras Synthesis of In-Situ Carbon Coated Lithium Iron Phosphate Using Low-Cost Iron Precursors for Lithium-Ion Batteries

10:30-11:00 Coffee Break and Poster Session at SSCU Foyer

Session – V: Session Chair: Session Chair 5 11:00-11:30 *Marie Guignard,* ICMCB, Bordeaux Designing new lithium layered oxides from sodium layered oxides

11:30-12:00 **A. Sundaresan,** JNCASR, Bangalore Multiferroic properties in the polar magnets  $LuMWO_{6}$  (M = Fe, Cr) 12:00-12:30 Sheetal Kumar Jain, IISc Bangalore

Triangulating Mn(II) Insertion in Cs2NaBiCl6 Doped Double Perovskite using Magnetic Resonance Spectroscopy

12:30-12:45 Krishna Kaushik, IISc Bangalore

Reversible Crystal-to-Crystal Transformation Associated with Photo and Thermo-Induced Metal-to-Metal Electron Transfer In Heterobimetallic 2D Network

12:45-14:00 Lunch at and Poster Session at SSCU Foyer

Session – VI Session Chair: Session Chair 6 14:00–14:30 Naga Phani Aetukuri, IISc Bangalore Batteries for Carbon Neutral Energy Transition

14:30–15:00 *Sebastian Peter,* JNCASR, Bangalore Exploiting Structural Orderness in Intermetallics to Discover Economical Catalysts for their Applications in Energy and Environmental sectors

15:00-15:30 *Ravishankar Narayan,* IISc Bangalore Insights into Nanostructure Growth, Structure and Stability Using Advanced Electron Microscopy

15:30-15:45 **Sunil Kumar,** IISc Bangalore Mechanism of Mg<sup>2+</sup> Mediated Encapsulation of an Anionic Cognate Ligand in a Bacterial Riboswitch

15:45–16:00 *Cyril Aymonier,* ICMCB Bordeaux The Institute for Condensed Matter Chemistry of Bordeaux

16:00-16:30 Concluding Session

16:30 Lab tour and Interaction

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## **Collaborations with France and CNRS: Opportunities and Mechanisms**

Srini Kaveri CNRS Email: <u>srini.kaveri@cnrs.fr</u>

The societal challenges such as health issues, demographic change, climate change, need for clean and efficient energy, smart and integrated transport, food security, and the bio-based economy, are all global. Addressing these challenges warrants answers that are also ought to be global and more importantly, there is a need for urgent solutions. An efficient international cooperation assisting a link between basic scientific research and industrial leadership is an absolute necessity to address these tasks. We will discuss the initiatives that the **French government** and **CNRS** present to support and enhance the scientific collaborations to address the societal challenges.

## Mixed Dimensional Heterostructures: a promising platform to explore innovative Advanced Materials and Devices

Dr. Jean–François Dayen Université de Strasbourg Institut de Physique et Chimie des Matériaux de Strasbourg, CNRS. Institut Universitaire de France, IUF. Email: dayen@unistra.fr

Illustrations of MWH that will be discussed for (a) optoelectronics, (b) magnetic molecular electronics.



Because of their atomically-thin structure, high surface-to-volume ratio, and reduced electric screening, new properties and functionalities are expected to emerge when exploiting the interactions of two-dimensional ('2D') materials placed in contact with other nanomaterials such as quantum dots, magnetic molecules or magnetic/ferroelectric thin films. These so-called *Mixed-dimensional van der Waals Heterostructures* ('MWH') are now at the forefront of basic nanoscience and applied nanotechnology, providing new sets of possibilities to tailor device functions and explore original physical properties.[1]

Today, I will present some of our recent achievements and ongoing works illustrating the possibilities offered by MWH in various fields of nanoelectronics including single-electron electronics [2], molecular electronics[3], spintronics [4], and optoelectronics[5].

The selected results will allow illustrating how fundamental & technological locks can be lifted by taking advantage of the functionalities of the nanomaterials (electronic, magnetic, optic...) and of the specific properties of 2D materials such as : i) van der Waals interface for nanomaterial growth/ interfacing, ii) dual electric behavior combining in-plane charge transport with out-of-plane electric field transparency (they are thinner than their screening length), iii) exacerbated surface/interface sensitivity for sensing.

Jariwala et al., Nat. Mater. 2017, 16, 170 ; [2] Mouafo <u>et al</u>, Adv. Mater. 2018, 30, 1802478; Mouafo <u>et al</u>., Adv.Func. Mat. 2021, 31, 2008255 ; Godel <u>et al</u>., Adv. Mater. 2017, 29, 1604837; [3] Konstantinov <u>et al</u>., J. Mat. Chem. C. 2021, 9, 2712 ; <u>Dayen</u> et al. Mater. Horiz., 2021, 8, 2310 ; [4] Godel <u>et al</u>., Appl. Phys. Lett. 2014, 105, 152407; <u>Dayen</u> et al., App. Phys. Rev. 2020, 7, 011303; [5] Noumbe <u>et al</u>., ACS Nano 2020, 14, 4567.

## Glass-like Thermal Conductivity in a Single Crystal of Layered Metal Halides

Kanishka Biswas

New Chemistry Unit, International Centre for Materials Science and School of Advanced Materials, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur P.O., Bangalore 560064 (India)

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As the periodic atomic arrangement of a crystal is made to a disorder or glassy-amorphous system by destroying the long-range order, the value of lattice thermal conductivity, KL, decreases, and its fundamental characteristics changes. Disordered atomic arrangement severely limits the phonon mean free path in a material, however, it can also have deteriorating effect on the charge carrier transport. Therefore, the realization of ultralow and unusual *glass-like* KL in a *crystalline* material is challenging but it holds the key to many applications like in thermoelectrics, thermal barrier coatings and hot phonon bottle neck in optoelectronics.<sup>1, 2</sup> I will be talking about achieving an ultralow value (~0.20 W/m·K at room temperature) and unusual glass-like temperature dependence (2-400 K range) of κL in a large single crystal of layered halide perovskite.<sup>3</sup> Soft acoustic phonons with low cut-off frequency (20 cm<sup>-1</sup>) are responsible for the low sound velocity in layered halide and makes the structure elastically soft with low bulk and shear moduli. While a strong anharmonicity originates from the low energy and localized rattling-like vibration of Cs atoms, synchrotron X-ray pair-distribution function analysis evidences the presence of a local structural distortion in the Bi-halide octahedra. We propose that the hierarchical chemical bonding and low energy vibrations from selective sublattice in the crystalline inorganic halide perovskites open an exciting platform for thermal transport research, which is intriguing from lattice dynamical aspects as well as have potential applications.

- 1. P. Acharyya, T. Ghosh, K. Pal, K. Kundu, K. S. Rana, J. Pandey, A. Soni, U. V. Waghmare and K. Biswas, *J. Am. Chem. Soc.*, 2020, *142*, 15595.
- 2. T. Ghosh, M. Dutta, D. Sarkar and K. Biswas, *J. Am. Chem. Soc.* 2022, 144, 10099.
- P. Acharyya, T. Ghosh, K. Pal, K. S. Rana, M. Dutta, D. Swain, M. Etter, A. Soni, U. V. Waghmare and K. Biswas, *Nat. Commun.* 2022, 13, 5053.

#### Circular chemistry in supercritical fluids for advanced functional materials

Cyril Aymonier, Marie Claverie, Marta Diez Garcia, Fransisco Aguirre, Gilles PhilippotInstitut for Condensed Matter Chemistry of Bordeaux 87 Avenue du Dr Albert Schweitzer, 33608 Pessac Cedex, France Email:cyril.aymonier@icmcb.cnrs.fr



The specific properties of supercritical fluids are exploited for more than 35 years to develop breakthrough technologies, especially in the field of the preparation of advanced materials, from organics to inorganics through carbon-based materials. This process of material design is continuous, fast (few tens of seconds), sustainable and scalable and gives access to high quality nanostructured materials with unique physico-chemical properties, meaning which

cannot be obtained with other synthetic methods.

This presentation proposes to introduce first the the experimental and modelling tools developed by chemists, chemical engineers, material chemists, physicists, *etc.*, which are today available to synthesize, shape and recycle materials.

After, this presentation will emphasize how the coupling between chemistry and chemical engineering gives access to the formation of unique and high quality nanostructured materials. For instance, the first proof of the synthesis in few tens of seconds of geominerals, namely talc, in a continuous millifluidic process will be presented. Very interestingly, this synthetic talc exhibits unique properties as its hydrophilicity knowing that naturel talc is hydrophobic. In this new field of geomineral synthesis, we went one-step forward with the demonstration of the possibility to prepare highly crystalline geominerals in just few seconds again but under thermodynamically metastable conditions with the synthesis of the torbermorite mineral which is not abundantin nature but very interesting in the construction industry for the development of green concretes. The mastering of the chemistry coupled with one pot multi-step processes opens the road towards the continuous design of multifunctional materials as illustrated with functional layer double hydroxides. All these materialscan now be produced from laboratory scale for research & development investigations to pilot scale for industrial purposes.

This presentation will also demonstrate the added value of the supercritical solvothermal synthesis methodin terms of materials. This will be illustrated with different examples in the fields of optics, energy, catalysis and microelectronics.

The benefits of the sub- and supercritical continuous solvothermal route include not only better performances for advanced applications but also environmental issues associated with the synthesis process. This will be emphasized with the studies performed using LCA approaches coupled with risk assessment ones. Finally, mastering physicochemistry and processes in supercritical fluids opens the way of a circular economy offering innovative solutions for the recycling of materials. This will be illustrated with the recycling of solar panels, permanent magnets, carbon fibers from CFRP, batteries or still the regeneration of chirurgical and FFP2 face masks.

## METAVALENT BONDING ORIGINS OF Unusual Properties of Group IV Chalcogenides

Umesh V. Waghmare

### Hydroxysulfates as cathode materials for rechargeable batteries

Shashwat Singh<sup>a\*</sup>, Valérie Pralong<sup>b</sup>, and Prabeer Barpanda<sup>a</sup> <sup>a</sup>Faraday Materials Laboratory, Materials Research Centre, Indian Institute of Science, Bangalore – 560012, India <sup>b</sup>Normandie University, Ensicaen, Unicaen, CNRS, Crismat, 14000 Caen, France Email: <u>shashwats@iisc.ac.in</u>

Hydroxysulfate (AMSO<sub>4</sub>OH) compounds form a niche class of high-voltage polyanionic battery cathodes with a desirable combination of efficient electrochemical activity along with moisture resistance due to the presence of hydroxyl (OH) group<sup>1</sup>. Monoclinic FeSO<sub>4</sub>OH (s.g. C2/c) was the first reported hydroxysulfate cathode exhibiting an  $Fe^{3+}/Fe^{2+}$ redox potential at 3.2 V with capacity over 120 mAh/g involving a two-step biphasic redox reaction<sup>2,3</sup>. Showcasing its versatility, here we report the first demonstration of reversible Na<sup>+</sup> (de)insertion in FeSO₄OH via single step biphasic reaction at ~2.9 V with a discharge capacity of 85 mAh/g. The size of (de)intercalating ions can trigger varied structural/ electrochemical properties in addition to polymorphism<sup>4</sup>. In this pursuit, an orthorhombic polymorph of FeSO, OH (s.g. Pnma) has been investigated for the first time focusing on its electrochemical performance. When implemented as cathode for Li-ion battery, it delivered a reversible capacity of 105 mAh/g (0.66 Li<sup>+</sup>) at C/20 with  $Fe^{3+}/Fe^{2+}$  redox potential centered ~3.2 V (vs Li/Li<sup>+</sup>). Deviating from monoclinic form, the orthorhombic FeSO<sub>4</sub>OH underwent a monophasic redox mechanism. This presentation will discuss (i) the first reports of FeSO, OH hydroxysulfate as cathodes for post Li-ion (Na-ion) batteries, (ii) the first demonstration of orthorhombic FeSO, OH as an economic air-stable cathode for Li-ion and Na-ion batteries, and (iii) in-depth mechanistic understanding of the electrochemical redox reaction in both orthorhombic and monoclinic polymorphs of FeSO<sub>4</sub>OH cathodes. This work will showcase synergistic study of hydroxysulfate cathodes using in-operando analytical tools, electrochemical titration techniques and first-principle (DFT) calculations.

- 1. S. Singh, S. Lochab, L. Sharma, V. Pralong, P. Barpanda, *An overview of hydroxy-based polyanionic cathode insertion materials for metal-ion batteries*, Phys. Chem. Chem. Phys. 23 (2021) 18283–18299.
- 2. M. Anji Reddy, V. Pralong, V. Caignaert, U.V. Varadaraju, B. Raveau, *Monoclinic iron hydroxy sulphate: A new route to electrode materials*, Electrochem. Commun. 11 (2009) 1807–1810.
- 3. M. Ati, M.T. Sougrati, G. Rousse, N. Recham, M.L. Doublet, J.C. Jumas, J.M. Tarascon, Single-Step Synthesis of  $FeSO_4F_{1-y}OHy$  ( $0 \le y \le 1$ ) Positive Electrodes for Li-Based Batteries., Chem. Mater. 43 (2012) 1472–1485.
- M. Ben Yahia, F. Lemoigno, G. Rousse, F. Boucher, J.M. Tarascon, M.L. Doublet, Origin of the 3.6 V to 3.9 V voltage increase in the LiFeSO<sub>4</sub>F cathodes for Li-ion batteries, Energy Environ. Sci. 5 (2012) 9584–9594.

## Near-IR organic photodetector

Neha Chauhan



## Unraveling the Novel Magnetic Properties of Columbites: An Emphasis on the Tricritical Point in H-T Phase diagram

<u>Subhash Thota</u><sup>a\*</sup> and Mohindar Singh Seehra<sup>b</sup> <sup>a</sup>Department of Physics, Indian Institute of Technology Guwahati, 781039, Assam, India <sup>b</sup>Department of Physics & Astronomy, West Virginia University, Morgantown-26506(WV), USA

The quest for discovery of real systems whose measured properties can be utilized to check the predictions of mathematical-models in condensed matter physics is very much needed nowadays because such comparisons provide great insight into underlining physics of microscopic world [1]. One such recent case is the predictions of excitations near a quantum critical point, which have beenrecently tested in the ferromagnetic Ising-chain columbites like CoNb<sub>2</sub>O<sub>6</sub> and NiNb<sub>2</sub>O<sub>6</sub> [2-4]. In this direction, the present talk is focused on the unique magnetic properties of few transition metal (M) Niobates (Mb,O<sub>6</sub>). These compounds usually crystallize in the columbite structure of space group  $D^{14}$  -Pbcn with orthorhombic unit cell containing four molecules per unit cell. Most often the crystalstructure of these compounds can be treated as zig-zag chains of divalent transition metal ions along the c-axis (Isinglike). Effectively the unit-cell contains two crystallographically inequivalent M<sup>2+</sup> ions and isosceles triangular arrangement of M<sup>2+</sup> ions in the ab plane. Rich details of the H-T phase diagram mapped using various phase transitions including the fieldinduced spin-flop transitions together with the intrachain  $(J_{a})$  and interchain  $(J_{1})$  and J<sub>2</sub>)) exchange interactions of few columbite structures will be discussed.

- 1. S. Sachdev, Quantum Phase Transition (Cambridge University Press, Cambridge, 1999).
- 2. S. Thota, et. al. Phys. Rev. B. 2021, 103, 064415.
- 3. R. Maruthi, et. al. J. Phys: Condens. Matter. 2022, 34, 155801.
- 4. R. Maruthi, et. al. J. Phys: Condens. Matter. 2021, 33, 345801.

#### Multifunctional hybrid layered materials: synthesis and structure - property relationships

Pierre Rabu

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Chemical and structural versatility of layered metal hydroxides and oxides allows for insertion and grafting of various kinds of functional molecules in between magnetic or ferroelectric sheets. This ability is promising for generating multi-functionality. Numerous properties can be combined as conductivity, luminescence, chirality, magnetism electro-activity, catalysis, etc In addition, these functionalities can be rather easily modulated by changing the host structure as well as the inserted species. Such "Lego©" chemistry seems really appropriate and we obtained many magnetic (2D-3D), magneto-luminescent and magneto-electric systems.<sup>1,2</sup> Although successful, this approach is still quite serendipitous and a better control *a priori* of the synthesis and precise knowledge of the structure of these hybrid materials are necessary to help the designing of new layered hybrids.

We present here recent results concerning magnetic and multifunctional layered hydroxides (LSH) and oxides (aurivillius) illustrating the mechanisms involved in insertion-grafting reactions, up to exfoliation. Our results enlarge the library of molecular species that is possible to graft into inter-lamellar space using various activation conditions.<sup>2–5</sup> We will describe efficient structural characterization techniques and analytical tools (TEM, XRD analysis and modeling) that were developed to investigate the structural features of these systems, allowing for establishing structure-

properties relationships, together with improvement of the design of layered functional materials. Acknowledgements: CNRS, University of Strasbourg, Région Grand Est, contract No. ANR-14-CE07-0004-01 (HYMN)) and the Labex NIE (ANR-11-LABX-0058\_NIE within the Investissement d'Avenir program ANR-10-IDEX-0002-02).

- (1) Rabu, P.; Delahaye, E.; Rogez, G. Hybrid Interfaces in Layered Hydroxides: Magnetic and Multifunctional Superstructures by Design. *Nanotechnol. Rev.* **2015**, *4* (6), 557–580. https://doi.org/10.1515/ntrev-2015-0017.
- Evrard, Q.; Chaker, Z.; Roger, M.; Sevrain, C. M.; Delahaye, E.; Gallart, M.; Gilliot, P.; Leuvrey, C.; Rueff, J.-M.; Rabu, P.; Massobrio, C.; Boero, M.; Pautrat, A.; Jaffrès, P.-A.; Ori, G.; Rogez, G. Layered Simple Hydroxides Functionalized by Fluorene-Phosphonic Acids: Synthesis, Interface Theoretical Insights, and Magnetoelectric Effect. *Adv. Funct. Mater.* 2017, *27* (41), 1703576. https://doi.org/10.1002/adfm.201703576.
- Evrard, Q.; Leuvrey, C.; Farger, P.; Delahaye, E.; Rabu, P.; Taupier, G.; Dorkenoo, K. D.; Rueff, J.-M.; Barrier, N.; Pérez, O.; Rogez, G. Noncentrosymmetric Cu(II) Layered Hydroxide: Synthesis, Crystal Structure, Nonlinear Optical, and Magnetic Properties of Cu2(OH)3(C12H25SO4). *Cryst. Growth Des.* 2018, 18 (3), 1809–1817. https://doi.org/10.1021/acs.cgd.7b01692.
- (4) Wang, Y.; Leuvrey, C.; Delahaye, E.; Leroux, F.; Rabu, P.; Taviot-Guého, C.; Rogez, G. Tuning the Organization of the Interlayer Organic Moiety in a Hybrid Layered Perovskite. J. Solid State Chem. 2019, 269, 532–539. https://doi. org/10.1016/j.jssc.2018.10.034.
- (5) Payet, F.; Bouillet, C.; Leroux, F.; Leuvrey, C.; Rabu, P.; Schosseler, F.; Taviot-Guého, C.; Rogez, G. Fast and Efficient Shear-Force Assisted Production of Covalently Functionalized Oxide Nanosheets. J. Colloid Interface Sci. 2022, 607, 621–632. https://doi.org/10.1016/j.jcis.2021.08.213.

### Multidimensional Electronic Spectroscopy with Combined Spectral, Temporal, and Spatial Resolution

Vivek Tiwari<sup>a\*</sup> FG14, Solid State and Structural Chemistry Unit, Chemical Sciences Building, Indian Institute of Science Bangalore Email: <u>vivektiwari@iisc.ac.in</u>

Controlling exciting state photophysics and reaction outcomes through excited state quantum coherences that leverage coupled vibrational-electronic motions is an emerging area of interest among spectroscopists and synthetic chemists alike. With advent of new molecular design strategies, development of new spectroscopic methods that can probe and unambiguously decongest the coupled motions of vibrations and electronics becomes imperative.

In this talk I will present our recent efforts towards development of a novel spectroscopic tool, *Multidimensional Electronic Spectroscopy* (MES) that decongests the femtosecond quantum dynamics of vibrations and electrons along three spectroscopic dimensions – excitation, detection and coherence frequency axes. The spatial resolution of this method is only limited by the microscope objective. Using fluorescence-detection, we demonstrate near 2-3 orders of magnitude sensitivity enhancement in *fMES*, compared to conventional MES techniques. Sensitivity enhancement is demonstrated by the ability to isolated excited state vibrational quantum beats based on the phase of quantum beating. Our approach paves the way for high-sensitivity probing of vibronic coupling and subsequent energy/charge transfer quantum dynamics in synthetically tailored donor-acceptor systems.



**Figure** – *fMES* spectra of a laser dye Oxazine 720 at room temperature. (left) 2D spectra at pump-probe waiting time T = 0 and 3 ps showing evolving femtosecond polar solvation dynamics. (right) Excited State vibrational quantum beats, shown as 2D coherence map, accompanying the polar solvation process isolated at ODs ~2-3x lesser than conventional MES approaches.

## Magnetocaloric Effect in (111) Oriented La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> – SrRuO<sub>3</sub> Superlattices

Prahallad Padhan,<sup>a,\*</sup> Roshna S. H.,<sup>a</sup> and W. Prellier<sup>b</sup> <sup>a</sup>Nanoscale Laboratory, Department of Physics, Indian Institute of Technology Madras, Chennai-600036, Tamil Nādu, India <sup>b</sup>Laboratoire CRISMAT, CNRS UMR 6508, ENSICAEN, 6 Bd du Marechal Juin, F-14050 Caen Cedex, France Email: padhan@iitm.ac.in

Magnetocaloric effect (MCE), i.e., reversible temperature change experienced by a magnetic material upon the application or removal of a magnetic field, has attracted much attention because it offers an energy-efficient and environment-friendly alternative to refrigeration technology.<sup>1</sup> The MCE of several magnetic materials has been characterized in bulk, nanoparticles, thin film and superlattice form. The properties of thin films or superlattice as compared to their bulk counterparts vary widely depending on the chemical composition, substrate, thickness, oxygen content, etc., of oxide materials. The study of field and temperature-dependent magnetization in  $La_{0.7}Sr_{0.3}MnO_3 - SrRuO_3$  superlattices indicates that the enhanced MCE can be achieved in the strained rather than relaxed superlattice.<sup>2</sup> The spin disordered–to–ordered transition in superlattices triggers the spin-phonon coupling, which appeared as an anomaly in the temperature-dependent Raman parameters. The presence of softer spin disorder requires a smaller range of thermal energy  $\Delta T$  (change in temperature) for the occurrence of transition from paramagnetic state to ferromagnetic state, thus, reducing the relative cooling power in the superlattice.



Figure 1Temperature-dependent phonon frequency shifts and change in magnetic anisotropy of the (111) oriented $La_{0.7}Sr_{0.3}MnO_3 - SrRuO_3$  superlattices.

- 1. N. A. Mezaal, K. V. Osintsev and T. B. Zhirgalova, *IOP Conf. Ser. Earth Environ. Sci.*, 2017, 87, 1.
- 2. Roshna S. H., W. Prellier and P. Padhan, Nanoscale, 2020,12, 5151.

# Microscopy of Engineered Area Nanostructures

Subham Kumar Saha

# Design of new ionic conductor used as electrode or solid electrolyte for non-aqueous batteries

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One of the major challenges of the 21<sup>st</sup> century is our ability to solve energy-related problems caused by ever-higher consumption, demography and standard of living. It is therefore imperative to anticipate this energy demand and this in a context of sustainable development. Storage technologies are highly dependent on the materials used and it is necessary to search for new materials with advanced properties that are also ecological and economical. Despite the high performance of lithium-based materials, its cost is driving scientists to develop alternative systems based on sodium and potassium, which are widely abundant in the earth's crust.

Manganese based oxide materials are promising cathodes for alkaline ion batteries due to their high energy density, low-cost and low-toxicity. Focusing on layered-type structures, one has to cite of course the A, MnO, families showing interesting insertion properties in all the system based on lithium, sodium and even more recently potassium. Moreover, we notice that the system A-Mn-O are extremely rich in term of original structures. For example, we found a new lithium rich composition Li<sub>4</sub>Mn<sub>2</sub>O<sub>5</sub> with a disordered rock salt structure that was showing an exceptional capacity of about 300mAg/g. Interestingly, the material  $Na_4Mn_2O_5$  has been reported with a layered type structure, different from the lithiated phase and we will discuss the relationship between the structure and insertion properties. In addition, with the aim of making lithium batteries safer, the scientific community is looking in recent years to replace the liquid solvents used as electrolyte with a solid ionic conductor compound. Thus, new materials ionic conductors are needed. Several families of materials have been developed, leading to major improvements in this technology (NASICON, perovskites, Garnets). In addition, the thio-phosphate family is widely explored and several compounds have been discovered in the pseudo-binary Li<sub>2</sub>S-P<sub>2</sub>S<sub>5</sub> diagram such as Li<sub>3</sub>PS<sub>4</sub>, Li<sub>7</sub>P<sub>3</sub>S<sub>11</sub> or Li<sub>7</sub>PS<sub>6</sub> In 2011, R. Kanno and al. had discovered a new phase: Li<sub>10</sub>GeP<sub>2</sub>S<sub>12</sub> showing ionic conduction of 12 mS/cm. Unfortunately, this structure is unstable towards lithium metal and germanium remains a very expensive element. In order to improve the stability of this structure, a partial substitution of sulfur by oxygen has been successfully obtained and shown better cycling capability. Very recently, the germanium-free phase  $Li_{9.6}P_{3}S_{12}$  has been obtained and exhibits better stability towards lithium despite a lower conductivity.

In this presentation, we will discuss the structure –properties relationship for these phases and detail our strategy to design a suitable ionic conductor.

# Berry curvature dipole in two-dimensional materials

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In recent years, it has been discovered that inversion symmetry broken quantum systems can exhibit non-linear Hall effect even under time-reversal symmetric conditions [1]. The underlying quantum object leading to this effect is the first order moment of the Berry curvature, termed the Berry curvature dipole. Such non-linear Hall effects open up different possibilities for direct applications, such as non-linear photocurrents and terahertz radiation detection [2]. However, despite such promise for exciting physics and applications, the Berry curvature dipole induced nonlinear Hall effect has been experimentally realized only in a handful of materials. It is, therefore, of vital importance to find materials with large and controllable Berry curvature dipole.

In this talk, I will give two examples from our work where such a controllable Berry curvature dipole has been predicted. First, we propose Janus monolayers of transition metal dichalcogenides as a promising materials platform to explore the non-linear Hall effect and Berry curvature dipole physics [3]. Here the topology and the Berry curvature dipole are tunable by chemical composition. Second, we discover a giant non-linear Hall effect in the elemental buckled honeycomb lattices -- silicene, germanene, and stanene [4]. In this case, the Berry curvature dipole is tunable by a transverse electric field which breaks inversion symmetry. We demonstrate that the electric field induced topological phase transitions are associated with a giant Berry curvature dipole near the critical field.

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## Synthesis of In-Situ Carbon Coated Lithium Iron Phosphate Using Low- Cost Iron Precursors for Lithium-Ion Batteries

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In the current scenario, Lithium-ion batteries (LIB's) play an important role for mobility and storage applications. In this context, lithium iron phosphate (LFP) is a well known cathode material in LIB's. Due to its inherent safety and low cost, the demand for LFP is high for current LIB's. The conventional method for preparing lithium iron phosphate is solid-state synthesis, but it can also be prepared by wet chemical route. The former approach provides micron-sized particles whereas, the latter approach yields nanoparticles. In general, to synthesize the LFP powder, precursors such as iron (II) acetate or iron (II) oxalate are used as iron source. These precursors are expensive and eventually increase the cost of the battery. Thus, to decrease the cost of the battery alternate precursors need to be explored for LFP synthesis.

Presently, a solid-state reaction approach has been adopted for LFP synthesis. Iron oxide (Fe<sub>2</sub>O<sub>3</sub>) is used as precursor along with iron powder in order to reduce the oxidation state from Fe (III) to Fe (II) of iron oxide. Apart from the iron precursor, lithium carbonate, ammonium dihydrogen phosphate and sucrose are used for synthesizing LFP. Sucrose acts as a reducing agent as well as source of conductive carbon additive for LFP. The obtained powder is single phase LFP. The particlesize ranges from ~20 to 30  $\mu$ m. To reduce the particle size of LFP, jet milling of the micron-sized powder has been carried out. Further, both as-synthesized and jet milled powders are tested for electrochemical performance in half-cell mode with lithium metal as anode using Swagelok cells at 0.1C rate for 100 cycles. The specific capacities obtained are reasonable *vis-a'-vis* values obtained using other synthesis procedures. Moreover, the prepared LFP powder is economical as well as feasible for LIB applications. The details of synthesis, characterization and electrochemical performance of the LFP powders will be presented.

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#### Designing new lithium layered oxides from sodium layered oxides

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Lithium-ion technology is the most promising avenue for the electrification of vehicles. Although already currently in use for several decades, an optimization of the electrode materials is still possible. In this context, lithium-rich layered oxides  $Li_{1+x}M_{1-x}O_2$  (where 0 < x < 1/3, and M is usually a mix of manganese, nickel and cobalt) have been intensively studied as positive electrode materials in lithium-ion batteries due to their high capacity (more than 250 mAh/g). However, these materials also present some serious drawbacks. Batteries made with these materials at the positive electrode can show an important capacity loss after the first cycle due to the partial irreversibility of the oxygen redox process. They also exhibit a decrease in voltage during cycling which originates with the migration of manganese ions within the lithium layers and the formation of a spinel-like structure at the surface of the particles.

To overcome these problems, we decided to synthesize new lithium-rich layered oxides with the general formula  $Li_{1,y}Mn_{1,y}O_2$  (with 0 < x < 0.25) with a different oxygen stacking that would make the migration of manganese ions unfavourable thanks to a stronger coulombic repulsion between the layers (alternative of face- and edge-sharing LiO<sub>6</sub> and MO<sub>6</sub> octahedra). The O6type lithium-rich layered oxide O6-LiNi $_{1/6}$ Mn $_{4/6}$ O $_2$  was obtained by ion exchange from the P2-type sodium layered oxide P2-Na<sub>5/6</sub>Li<sub>1/6</sub>Ni<sub>1/6</sub>Mn<sub>4/6</sub>O<sub>2</sub>. In a first step, the ion exchange was monitored by variable temperature X-ray diffraction and we observed that an intermediate compound was formed during the ion exchange reaction. X-ray diffraction suggested that this compound was a layered oxide, alternating layers of sodium ions located in prismatic sites and layers of lithium ions located in octahedral sites, these two layers being separated by a layer of MO6 octahedra (where M is Li, Ni and Mn). At the end of the ion exchange reaction, a pure lithium layered oxide is obtained with no remaining sodium. Its structure was studied by coupling X-ray and neutron diffraction and high-resolution transmission electron microscopy. We concluded that the layered structure was not a pure O6-type structure and that some stacking faults existed (about 15 %). Finally, the O6-LiNi $_{1/6}$ Mn $_{4/6}$ O $_2$  compound was used as the positive electrode material in lithium batteries. The batteries were galvanostatically cycled between 2.6 and 4.6 V and they showed good capacities and capacities retention. The voltage plateau observed during the first charge at approximately 4.5 V seems to be related to oxygen oxidation. The good capacity retention suggests that the oxygen redox is at least partially reversible.

### Multiferroic properties in the polar magnets $LuMWO_{6}$ (M = Fe, Cr)

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We have investigated the magnetic structures and multiferroic properties of the isostructural polar compounds, LuFeWO<sub>6</sub> and LuCrWO<sub>6</sub>. Both compounds crystallize in the polar orthorhombic aeschynite type mineral structure (space group *Pna2*<sub>1</sub>) with the ordered Fe<sup>3+</sup>/Cr<sup>3+</sup> and W<sup>6+</sup> ions. DC magnetization data reveal the antiferromagnetic ordering of Fe<sup>3+</sup> spins at T<sub>N</sub> = 11.8 K in LuFeWO<sub>6</sub>, and the Cr<sup>3+</sup> spins ordering at T<sub>N</sub> = 19.2 K in LuCrWO<sub>6</sub>. Analysis of neutron diffraction data at 1.5 K for LuFeWO<sub>6</sub> show a noncollinear magnetic structure with **k** = (0, ½, ½), and for LuCrWO<sub>6</sub>, a collinear magnetic structure with **k** = (0, ½, ½), and for LuCrWO<sub>6</sub>, a collinear magnetic structure with **k** = (0, 0, 0). A dielectric anomaly and a change in polarization occur at T<sub>N</sub> in LuFeWO<sub>6</sub>, while no polarization is observed in LuCrWO<sub>6</sub>. It is suggested that the noncollinear magnetic structure is responsible for the multiferroicity in the Fe compound.



Figure 1 Magnetic structure of (a) LuFeWO<sub>6</sub> and (b) LuCrWO<sub>6</sub> at 1.5 K.

## Triangulating Mn(II) Insertion in Cs<sub>2</sub>NaBiCl<sub>6</sub> Doped Double Perovskiteusing Magnetic Resonance Spectroscopy

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Metal halide double perovskite materials are gaining increasing attention for optoelectronic applications. Transition metal-doped double perovskites are emerging as lead-free, stable semiconducting materials with tailorable optical bandgaps. One candidate material is Mn(II)-doped Cs2NaBiCl6, where the influence of Mn-insertion on the chemical structure is poorly understood due to Mn low loading. A comprehensive three-pronged strategy involving solid-state nuclear magnetic resonance (NMR), high field dynamic nuclear polarization (DNP), and electron paramagnetic resonance (EPR) spectroscopies to identify the location of Mn(II)-insertion in these materials will be presented. Complimentary EPR and NMR measurements will be shown to confirm that the cubic structure is maintained with Mn(II) incorporation at room temperature. Moreover, Paramagnetic Relaxation Effect (PRE) and hyperfine sublevel Correlation (HYSCORE) EPR spectroscopy results will be discussed that indicate that Bi-Mn exchange is preferred on doping. Finally, Endogenous DNP NMR measurements from Mn(II)  $\rightarrow$  <sup>133</sup>Cs (<30 K), revealing that the Mn(II) is homogeneously distributed within the double perovskite phase, will be shown.



**Figure 1** The Crystal structures of the Cs<sub>2</sub>NaBiCl<sub>6</sub> parent and possible local structural models forMn<sup>2+</sup> doped Cs<sub>2</sub>NaBiCl<sub>6</sub>. (b) Mn(II)-<sup>133</sup>Cs DNP profile (blue) overlayed with Mn(II) EPR spectrum recorded at 6.9 T at 15K. (c) Mn(II) HYSCORE-EPR spectrum collected at Q-band, 30K.

## Reversible Crystal-to-Crystal Transformation Associated with Photo and Thermo-Induced Metalto Metal Electron Transfer in Heterobimetallic 2D Network

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In the modern era of technology, considerable attention has been given to the materials that can reduce the size of electronic devices and can be used for high-density storage devices, quantum computing, spintronics, sensors etc.<sup>[1]</sup> Room temperature bistable materials, where the properties of the materials can be switched with the sight alternation of external stimuli are desirable for application purposes. In this regard, switchable magnetic materials based on metal-to-metal electron transfer (MMET) are promising and have been explored over the last few years.<sup>[2]</sup> Amongst them, a particular interest has been given to the materials designed using octacyanometallates ( $[M^{IV/V}(CN)^8]$  <sup>n-</sup> = W, Mo, Re) building blocks that can be used judiciously for the designing of multifunctional magnetic materials. These materials exhibit an enormous range of anticipated physical properties, including long-range magnetic ordering, photomagnetic effect, electro-magnetic properties etc.<sup>[3]</sup>



Figure: Crystal structure and  $\Box T$  vs T plot of 2D coordination Networks

Here in my talk, I will present the magnetostructural correlation of our recent work based on 2D coordination networks. The novel 2D coordination networks were designed by using octacyanometallates building block and nitrogen donor ligands on 3d metal side. The resulting 2D network uptake moisture and reversibly convert into another form. Detailed (photo)magnetic studies reveal that MMET occured in both the forms togethar with near room temperature large thermal hysteresis loops along with ferromagnetic ordering at low temperature. The novel materials

suggest new resource for magnetism in 2D extended corrdination networks. Acknowledgement: I thank Indian Institute of Science (IISc), Solid State and Structural Chemistry Unit (SSCU) for my research work and financial support.

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## **Batteries for Carbon Neutral Energy Transition**

Naga Phani Aetukuri

## Exploiting Structural Orderness in Intermetallics to Discover Economical Catalysts for their Applications in Energy and Environmental sectors

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Two most imminent scientific and technological problems that the mankind is facing now, is that of energy and climate. The energy production and utilization in modern society is mostly based on the combustion of carbonaceous fuels like coal, petroleum and natural gas the combustion of which produces CO2, which alters earth's carbon cycle. 30 billion of tons of CO2 per year get emitted globally as waste from the carbonaceous fuel burning and industrial sector, which if converted to valuable chemicals have the potential to change the economy of the world. We, in our lab are trying to address both issues and are keen upon translating our innovative technologies from the lab to the industrial and commercial scale. We are capturing CO2 from industrial flue stream (of any composition) and thermo- catalytically converting it to value added chemicals/fuels such as methanol, carbon-monoxide, methane, dimethyl ether, C2-C5 & C5-C11 gasoline hydrocarbons. Catalyst design is at the heart of all these technologies and we have developed customized catalyst systems for targeted product conversions as per the need of different industries.

In this talk, I will discuss about our recent discovery of three intermetallics as efficient catalysts: (1) industry level hydrogen production via electrochemical water splitting, (2) conversion of CO<sub>2</sub> to methanol electrochemically at low pressure and low potential and (3) complete electron transfer in the cathodic side of fuel cell. The talk will cover the development of the catalyst via various methods, the driving force behind the enhancement in activity and the mechanistic pathways by various insitu (DRIFTS, IR, XAFS), ex-situ (XPS, XRD, IR, XAFS) and theoretical (DFT calculation) studies. The talk also will cover the industrial viability of these catalysts. The talk is the summary of the following papers

- In-Situ Mechanistic Insights for Oxygen Reduction Reaction in Chemically Modulated Ordered Intermetallic Catalyst Promoting Complete Electron Transfer. Mondal, S.; Bagchi, D.; Sarkar, S.; Singh, A. K.; Vinod, C. P.; Peter, S. C. J. Am. Chem. Soc. 2022, 44, 11859–11869.
- Morphology Tuned Pt<sub>3</sub>Ge Accelerates Water Dissociation to Industrial Standard Hydrogen Production over a wide pH Range. Mondal, S.; Sarkar, S.; Bagchi, D.; Das, T.; Das, R.; Singh, A. K.; Prasanna, P. K.; Vinod, C. P.;
  Chakraborty, S.; Peter, S. C. *Adv. Mater*. 2022, 34, 2202294.
- Structure-Tailored Surface Oxide on Cu-Ga Intermetallics Enhances CO<sub>2</sub> Reduction Selectivity to Methanol at Ultra-Low Potential. Bagchi, D.; Raj, J.; Singh, A. K.; Cherevotan, A.; Roy, S.; Manoj, K. S.; Vinod, C. P.; Peter, S. C., *Adv. Mater.* 2022, 34, 2109426.

#### Insights into Nanostructure Growth, Structure and Stability Using Advanced Electron Microscopy

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Advanced electron microscopy techniques have become indispensable in our quest to make better materials for various applications. This is particularly true for energy materials where the TEM has played a key role in elucidating mechanisms of growth, stability and operation. In our group, we use advanced microscopy techniques to understand nucleation and growth mechanisms of nanostructures with particular emphasis on energy applications. In this talk, I will present several examples of porous structures, ultrathin nanowires, supported catalysts, single atom catalysts (SAC) and heterostructured materials for different applications. The emphasis will be on the microscopy technique that provides key insights in each case. Reaction-limited aggregation mechanism for porous structures, stability of nanoporous materials, controlling heterogeneous nucleation to obtain supported catalysts and SACs, nucleation texture in supported catalysts will be presented. A range of microscopy techniques including precession electron diffraction, in-situ heating, HAADF-STEM, EELS and tomography will be discussed.

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### Mechanism of Mg<sup>2+</sup> Mediated Encapsulation of an Anionic Cognate Ligand in a Bacterial Riboswitch

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The fluoride riboswitch is essential for bacteria's survival as it is critical to maintaining the F<sup>-</sup> ion concentration below the toxic level and is a target for antibiotic development. The anionic cognate ligand, F<sup>-</sup> ion, is encapsulated by three Mg<sup>2+</sup> ions in a trigonal pyramidal arrangement bound to the negatively charged ligand-binding domain (LBD) of the riboswitch. The assembly mechanism of this intriguing LBD structure and its role in transcription initiation are unclear. I performed computer simulations using coarse-grained and all-atom RNA models to bridge multiple timescales and show that F<sup>-</sup> and Mg<sup>2+</sup> binding is essential to stabilize the LBD structure and tertiary stacking interactions. The first two Mg<sup>2+</sup> ions bind to the LBD region through water-mediated outer-shell coordination even in the riboswitch unfolded state and should transition to a direct inner shell interaction through dehydration to strengthen their interaction with the LBD. I propose that the efficient binding mode of the third Mg<sup>2+</sup> and F<sup>-</sup> is they form a water-mediated ion pair and bind to the LBD simultaneously.

## The Institute for Condensed Matter Chemistry of Bordeaux

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The Institute for Condensed Matter Chemistry of Bordeaux (ICMCB - UMR 5026) is a Joint Research Unit of the CNRS, University of Bordeaux (UB) and Bordeaux INP.



Created in 1995 on the foundations of the former CNRS Solid Chemistry Laboratory, ICMCB the focused its research on Solid Chemistry, Materials Science, and Molecular Sciences. Today, the

synthetic and shaping control of compounds and materials requires an increasingly fine mastery of chemistry and therefore of the associated processes, which has led us to propose a new disciplinary field entitled Chemistry & Processes. Beyond the three unifying disciplinary areas, Solid State Chemistry, Materials Science, and Chemistry & Processes, the ICMCB aimsto enter the era of data science and artificial intelligence (AI) to accelerate the discovery of new compounds and materials and the development of sustainable processes.

Foundational to the laboratory, the field of "Condensed Matter" must be explored today in the context of "Resource Management", i.e., a limited and sustainable use of resources by minimizing the impact on the environment (limiting the use of toxic and critical elements, recycling and regeneration of materials, etc.) and the development of processes that conserve energy and resources. The eco-materials of tomorrow must be built with an anticipation of their end oflife and disassemble, in order to be part of a circular economy, from research to education and innovation.

The ICMCB project is part of the development of new concepts in the materials value chain, to synthesize, shape and recycle in a sustainable way new compounds and materials, or even compounds and materials with new properties, in order to meet the challenges of our society. Among the families of materials studied at the ICMCB, namely inorganic materials, inorganic-organic hybrid materials and molecular materials, emerging materials will emerge, in the hope that they will become innovative, in particular for energy, for sustainable development and for electronics and photonics.

The ICMCB actively participates in the structuring of research in the field of materials on the Bordeaux campus, at national, European and international levels. The laboratory is also strongly involved in industrial partnerships. A significant part of these collaborations is done with the active support of the "Région Nouvelle-Aquitaine" for which the ICMCB is one of the important partners of the public research effort. Finally, the ICMCB contributes significantly to the creation of companies.

While research requires culture and experience, it also needs creativity and dynamism. A large pool of young researchers is, in this context, a guarantee of success. Training young people, by and for research, is one of our essential missions. These young people thus trained will be the future managers of academic research, but also of R&D in industry.

## POSTER SESSION – MONDAY-TUESDAY, OCTOBER 03<sup>RD</sup>-04<sup>TH</sup>

Poster No	Poster Title	Author
P01	A Comparative Study of the Electrochemical Behavior of WO <sub>3</sub> and Li <sub>2</sub> WO <sub>4</sub> as Anodes for Lithium-Ion Batteries	U. V. Varadaraju
P02	ON/OFF Photo-Switching and Thermo- Induced Spin Crossover with Cooperative Luminescence in 2D Iron(II) Coordination Polymer	Sujit Kamilya
P03	Multidimensional Electronic Spectroscopy with Combined Spectral, Temporal, and Spatial Resolutions	Amitav Sahu
P04	Thermo and Photo-induced electron transfer in molecular model complexes of mixed valence Fe <sup>III</sup> /Fe <sup>II</sup> Prussian Blue	Sakshi Mehta
P05	Tunable topology and Berry curvature dipole in Janus monolayer derivatives of 1T' WTe <sub>2</sub>	Nesta Benno Jo- seph
P06	Pressure-induced magnetic and topological transitions in non- centrosymmetric MnIn <sub>2</sub> Te <sub>4</sub>	Anumita Bose
P07	Soil Characterization using Magnetic Resonance Spectroscopic Techniques	Nikita Rao



















