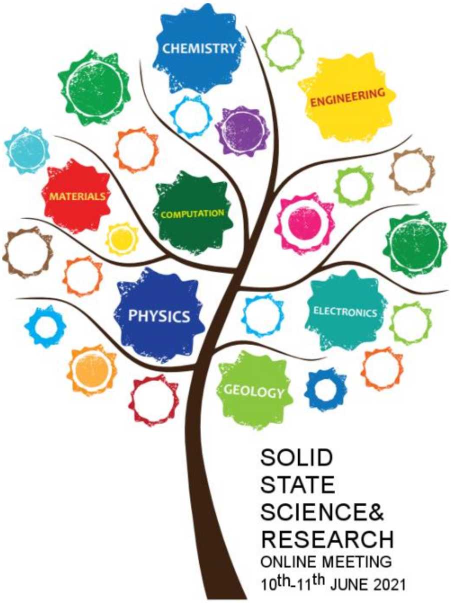
Book of Abstracts

10 & 11 June 2021, Zagreb, Croatia



SOLID
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10th-11th JUNE 2021

Solid-State Science & Research
Zagreb, 10 & 11 June 2021

BOOK OF ABSTRACTS AND PROGRAMME

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All times are in CEST (GMT+2)

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Keynote lectures

K01 - Crystal Engineering
Its Potential in Chemistry and Society

Gautam R. Desiraju[1]
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A field that was defined 30 years ago as "the understanding of intermolecular interactions in the context of crystal packing and in the utilisation of such understanding in the design of new solids with desired physical and chemical properties",[1] and which identified as the central issue in structure design the lack of a direct correspondence between molecular and crystal structure in the sequence "One → Few → Many → Nucleus → Crystal",[2] has now evolved into "in an area of virtually unlimited scope where science funding and translation efforts could be directed in the current climate of a society that increasingly expects applications and utility products from science and technology".[3] Certain current concerns will be addressed in this talk.

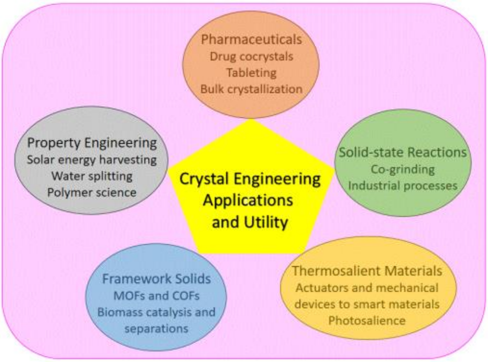

Figure 1 Five application domains of Crystal Engineering.

[1] G. R. Desiraju, *Crystal Engineering. The Design of Organic Solids,* Elsevier (1989).
[2] G. R. Desiraju, *J. Am. Chem. Soc.,* **135** (2013) 9952.
[3] A. K. Nangia, G. R. Desiraju, *Angew. Chem. Int. Ed.* **58** (2019) 4100.

K02 - Smart and Programmable Sponges for protection From Bench to Market

Omar K. Farha[1]
[1]Department of Chemistry, Northwestern University, Evanston, IL, USA
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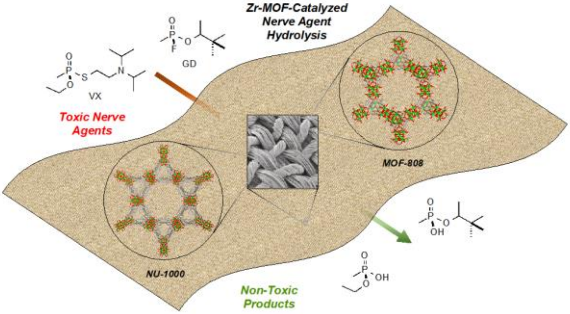
MOFs are a class of porous, crystalline materials composed of metal-based nodes and organic ligands that self-assemble into multi-dimensional lattices. In contrast to conventional porous materials such as zeolites and activated carbon, an abundantly diverse set of molecular building blocks allows for the realization of MOFs with a broad range of properties. We have developed an extensive understanding of how the physical architecture and chemical properties of MOFs affect material performance in applications such as catalytic activity for chemical warfare agent detoxification. This talk will focus on metal–organic frameworks (MOFs) for hydrolysis from solution-phase to solid-state reactivity. Moving MOFs from bench to market within industrial sectors will be discussed as well.



Invited lectures

I01 - The Rise of the Dynamic Crystals

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The anticipated shift in focal point of interest of solid-state chemists, crystal engineers and crystallographers from structure to properties to function of organic solids parallels the need to apply our accumulated understanding of the intricacies of crystal structure to explaining the related properties, with the ultimate goal of harnessing that knowledge in applications that require soft, light-weight, and/or biocompatible organic solids.[1] In these developments, the adaptive molecular single crystals warrant a particular attention as an alternative choice of materials for light, flexible, and environmentally benign devices, primarily memories, capacitors, sensors, and actuators. Some of the outstanding requirements for application of these dynamic materials as high-efficiency energy storage devices are strongly induced polarization, high switching field, and narrow hysteresis in case of reversible dynamic processes. However, having been studied almost exclusively by chemists, molecular crystals still lack the appropriate investigations that reliably evaluate their reproducibility, scalability, and actuating performance, and some important drawbacks have diverted the interest of engineers from these materials in applications. United under the umbrella term crystal adaptronics, the recent research efforts aim to realistically assess the appositeness of dynamic crystals for applications that require fast, reversible and continuous operation over prolonged periods of time. With the aim to highlight the most recent developments in the research of adaptive molecular crystals, this Perspective article discusses their assets and pitfalls. It also provides some hints on the likely future developments that capitalize on the untapped, sequestered potential for applications of this distinct materials class.

[1] P. Naumov, D. P. Karothu, E. Ahmed, L. Catalano, P. Commins, J. Mahmoud Halabi, M. B. Al-Handawi, L. Li, *J. Am. Chem. Soc.* **142** (2020) 13256.

I02 - How to Create Life from Dead Matter: Mechanisms to DNA, Molecular Evolution and Homochirality

Oliver Trapp[1]
[1]Department of Chemistry, Ludwig-Maximilians-University Munich, Munich
e-mail: oliver.trapp@cup.uni-muenchen.de

In this lecture I will present our research results and goals on the origin of life. First, I will concentrate on the formation of important simple chemical building blocks, which are formed by the catalytic effect of meteoric nanoparticles and the originally predominant earth atmosphere, namely hydrogen and carbon dioxide. We were able to show experimentally that traces of nanoparticles, which are created by the evaporation of meteorites when they enter the Earth's atmosphere, convert relatively inert carbon dioxide into interesting and highly reactive organic compounds.

Based on these compounds, we can follow the development of further important building blocks [1,2]. Recently, we achieved a decisive breakthrough in the prebiotic formation of DNA nucleoside building blocks [3,4]. Contrary to the opinion accepted by many scientists that an RNA world first developed that only produced DNA through complicated transformations, we have discovered a reaction pathway that leads directly to DNA. In the course of these investigations, we identified and characterized another DNA progenitor. These findings put us in a position to establish concrete conditions for the development of life. In this way we can explain why Nature prefers the sugar ribose or deoxyribose for RNA and DNA building blocks.

In a further part I will present a system for evolution on the molecular level, which will ultimately lead to the formation of "living chemical networks" [5,6].

[1] S. Lamour, S. Pallmann, M. Haas, O. Trapp, *Life* **9** (2019) 52.
[2] M. Haas, S. Lamour, S.B. Christ, O. Trapp, *Commun. Chem.* **3** (2020) 140.
[3] J.S. Teichert, F.M. Kruse, O. Trapp, *Angew. Chem. Int. Ed.* **58** (2019) 9944.
[4] F.M. Kruse, J.S. Teichert, O. Trapp, *Chem. Eur. J.* **26** (2020) 14776.
[5] O. Trapp, S. Lamour, F. Maier, A.F. Siegle, K. Zawatzky, B.F. Straub, *Chem. Eur. J.* **26** (2020) 15871.
[6] A.C. Closs, E. Fuks, M. Bechtel, O. Trapp, *Chem. Eur. J.* **26** (2020) 10702.

I03 - Extreme mechanics and viability of pollen grains

Antonio Šiber[1]
[1]Institute of physics, Bijenička cesta 46, 10000 Zagreb
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Pollen carries male plant genetic material encapsulated in a hard protective shell containing flexible, soft regions—apertures. The mechanical design of the shell regulates how the pollen grain folds into itself upon dehydration, which often occurs once it becomes exposed to the environment. The same design also guides the response of pollen grains to hydration which may lead to bursting of the pore and the leakage of the pollen proteins in the atmosphere – this process releases submicronic pollen particles, which can provoke strong allergic reactions in sensitive individuals. We investigate folding pathways of pollen grains by studying elastic deformations of inhomogeneous thin shells. Different pathways are governed by the interplay between the elastic properties of the hard and soft regions of the pollen shell and by the aperture shape, number, and size. We delineate regions of mechanical parameters of the pollen grain which lead to complete closure of all apertures, thus reducing water loss and presenting evolutionary viable solutions to the infolding problem [1]. We also show that the apertures, although important for the initiation of the pollen tube, also present a weak regions of the grain wall and that they are prone to bursting once the pollen grain swells enough in humid atmosphere [2].

[1] A. Božič, A. Šiber, *Proc. Natl. Acad. Sci. U.S.A.*. **117** (2020) 26600.
[2] A. Božič, A. Šiber, bioRxiv **2021**.05.24.445387

I04 - Plastic deformation, quantum-critical ferroelectric fluctuations and superconductivity in strontium titanate

Damjan Pelc[1,2]
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[2]School of Physics and Astronomy, University of Minnesota, USA
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Strontium titanate ($SrTiO_3$, STO) is one of the most studied transition metal oxides, with remarkable physical properties that have been debated for over five decades. It shows strong ferroelectric fluctuations, a highly controversial metallic state, and superconductivity at the lowest known charge carrier densities of any material [1]. However, it is less known that crystals of STO can be irreversibly, plastically deformed in an extremely wide range at ambient temperature. This provides the opportunity to study the effects of plastic deformation on the structural and electronic properties of a prototypical oxide. In this talk, I will show that plastic deformation of STO leads to self-organized dislocation structures (Fig. 1), which induce both quantum-critical ferroelectric fluctuations and a significant enhancement of the superconducting transition temperature [2]. I will discuss a simple explanation based on the coupling between local lattice strain and ferroelectricity, and argue that plastic deformation can be used as a novel way to tune the properties of quantum materials more generally.

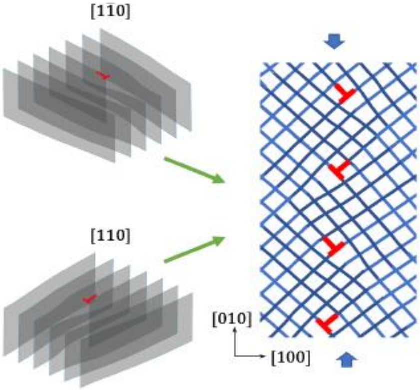

Figure 1 Self-organized dislocation walls in plastically deformed STO.

[1] C. Collignon et al., *Annu. Rev. Cond. Matter Phys.* **10** (2019) 25.
[2] S. Hameed et al., *arxiv:2005.00514* (2020).

I05 - Switching magnets with light: mechanisms and challenges

Andrei Kirilyuk[1]

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The manipulation of magnetization by light has grown into an active and intriguing area of research, driven by exceedingly urgent issues in information storage and processing. The ultrafast processes and non-equilibrium dynamics involved lead to intense discussions over possible mechanisms facilitating light-induced switching of magnetic order.

Previously, it has been demonstrated that the magnetization of ferrimagnetic RE-TM alloys and multilayers can be reversed by single femtosecond laser pulses [1,2]. The switching is however purely thermal and is actually driven by the ultrafast demagnetization of two ferrimagnetic sublattices, which naturally limits the application of the phenomenon.

Most exciting alternative to the thermal effects are the non-thermal ones such as opto-magnetic mechanism directly influencing the magnetization [3], or the photo-magnetic change of anisotropy, that is able to lead to ultrafast switching of magnetization in transparent magnetic dielectrics [4]. The polarization of the pulse determines the direction of switching. This mechanism outperforms alternatives in terms of the speed (<20 ps) and the unprecedentedly low heat load, making it attractive for possible applications.

As an outlook, an ultrafast modification of the crystal field environment and thus of magnetocrystalline anisotropy, may become the most universal way to manipulate the magnetization [5]. Magneto-elastic interactions are present in all materials and thus universal. We therefore discuss the application of this mechanism in antiferromagnets as well as other 'ferroics'.

[1] C.D. Stanciu, F. Hansteen, A.V. Kimel, A. Kirilyuk, A. Tsukamoto, A. Itoh, Th. Rasing, *Phys. Rev. Lett*. **99** (2007) 047601.

[2] A. Kirilyuk, A.V. Kimel, and Th. Rasing, *Rep. Prog. Phys*. **76** (2013) 026501.

[3] A.V. Kimel, A. Kirilyuk, P.A. Usachev, R.V. Pisarev, A.M. Balbashov, Th. Rasing, *Nature* **435** (2005) 655.

[4] A. Stupakiewicz, K. Szerenos, D. Afanasiev, A. Kirilyuk, A.V. Kimel, *Nature* **542** (2017) 71.

[5] A. Stupakiewicz, C.S. Davies, K. Szerenos, D. Afanasiev, K.S. Rabinovich, A.V. Boris, A. Caviglia, A.V. Kimel, A. Kirilyuk, *Nat. Phys.* **17** (2021) 489.

I06 - Characterization, control and manipulation of molecular spin ensembles by ESR

Vladislav Kataev
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Magnetically active metal-organic molecules that comprise in their cores interacting paramagnetic transition metal ions currently attract a significant interdisciplinary attention due to their unprecedented properties. Some of them provide realization on a molecular level of a superparamagnetic particle (single molecule magnet) characterized by a big and anisotropic magnetic moment, hysteresis behavior and metastable magnetic states. Such molecular-based materials provide a unique playground to study fundamental aspects of quantum magnetism on the macroscopic level but also there is a need to access them for possible applications in future spin electronic devices.

New techniques of tunable sub-Terahertz electron spin resonance spectroscopy in high magnetic fields (HF-ESR) enable detailed insights into the energy spectrum of the spin states, exchange interactions and anisotropy effects in such kind of systems. This will be illustrated in this talk by a few examples of HF-ESR studies of some representatives of this class of materials carried out at IFW Dresden. It will be shown how the spin-multiplet structure, magnetic anisotropy and exchange interactions can be assessed in the ESR experiment complemented by static magnetic measurements. A relationship between the chemical structure, bonding topology and magnetism of the studied compounds with regard to the rational design of functional materials will be briefly discussed.

I07 - Border Security: How to Detect Special Nuclear Material?

I.Capan[1], *J. Coutinho*[2], *L. Snoj*[3], *T. Makino*[4]
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[2]University of Aveiro, Aveiro, Portugal
[3]Jožef Stefan Institute, 1000 Ljubljana, Slovenia
[4]QST, Takasaki, Japan
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Increasingly complex risks, like geopolitical instability or decentralized terrorism threats, have led to the urge for deploying nuclear screening systems for detection of illicit trafficking of nuclear materials, and from that, to a growing interest in the field of research and development of new radiation detection technologies suitable for homeland security applications. Recent progress in the manufacturing of high-quality epitaxial silicon carbide (SiC) enables unprecedented detection properties of the future SiC-based detectors for neutron and alpha-particle emissions. Unlike existing and commonly used neutron gas-based detectors, SiC-based devices have the potential to be simultaneously portable, operable at room temperature and radiation hard. In this talk, we will present recently developed SiC detector prototype for efficient alpha-particle and thermal neutron detection.

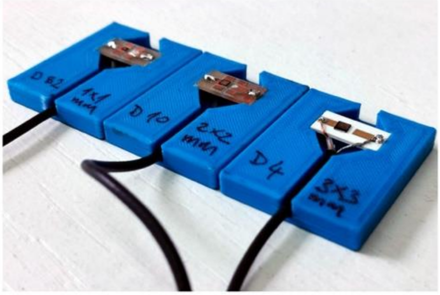

Figure 1 SiC detector prototype.

[1] I.Capan et al, *J. Appl. Phys.* **123** (2018) 161597.
[2] I.Capan et al, *J. Appl. Phys*. **124** (2018) 245701.

I08 - Point Defects in Functional Nano-Materials and Their Role in Energy Storage Devices

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Electron paramagnetic resonance (EPR) is a very powerful method due to its enhanced sensitivity to unpaired electrons. In order to understand the defect structure in functional nano-materials we use multi-frequency EPR spectroscopy. In this presentation i) quantum confinement effects in ferroelectric nano-materials ii) EPR and Photoluminescence (PL) investigations of intrinsic defect centers in semiconductor zinc oxide (ZnO) nanoparticles will be given iii) application of metal oxides as electrodes in supercapacitors will be discussed. Starting with the introductory information about EPR spectroscopy; poling, aging, doping and nano-size effects will be discussed for the ferroelectric materials such as, $PbTiO_3$, $BaTiO_3$, $PbZrTiO_3$ (PZT) etc. In the second part of the talk, surface and core defects and their reactivity under temperature and light will be presented for ZnO semiconductor nano-materials. Defect models will be discussed. Finally, in the last part designs of supercapacitor devices will be given and the role of defect structures in the electrochemical performance of supercapacitor devices will be presented.

Figure 1 Defect evolution of non-stoichiometric ZnO.

I09 - Mechanochemical and aging routes to nanoparticles and biopolymers

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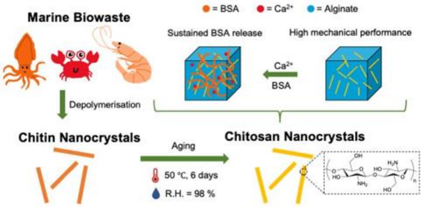
Mechanochemistry is becoming an established method for the sustainable, solid-phase synthesis of scores of nanomaterials and molecules, ranging from active pharmaceutical ingredients to materials for cleantech. In a first set of examples, we will look at ways with which it can be used to access nanoparticles of various metals [1,2], metals sulfides [3] and metal phosphides [4] with excellent control over their size, shape and size distribution. We will also discuss a structural-phase-field-crystal (XPFC) model with a ballistic driving force used as a means to gain insight into the growth of gold nanoparticles in a two-component mixture under mechanochemical conditions [5]. In a second set of examples, we will turn to the use of mechanochemistry and aging to access functional materials based on the chitin biopolymer. In particular, the use of these techniques will be shown for the conversion of chitin to chitosan [6], but also for the conversion of nanocrystals of chitin to nanocrystals of chitosan [7]. The latter materials feature superior properties in the context of hydrogel synthesis and are efficient ingredient for the device of slow drug release materials.



[1] M. J. Rak, N. K. Saadé, T. Friščić, A. Moores, *Green Chem*. **16** (2014) 86.
[2] M. Rak, T. Friščić, A. Moores, *RSC Adv*. **6** (2016) 58365.
[3] M. Malca, H. Bao, T. Bastaille, N. K. Saade, J. M. Kinsella, T. Friščić, A. Moores, *Chem. Mater*. **29** (2017) 7766.
[4] B. Fiss, N.-N. Vu, G. Douglas, T.-O. Do, T. Friščić, A. Moores, *ACS Sustain. Chem. Eng*. **8** (2020) 12014.
[5] L. Yang, A. Moores, T. Friscic, N. Provatas, *ACS App. Nano Mater*. **4** (2021) 1886.
[6] T. Di Nardo, C. Hadad, A. Nguyen Van Nhien, A. Moores, *Green Chem.* **21** (2019) 3276.
[7] T. Jin, T. Liu, S. Jiang, D. Kurdyla, B. A. Klein, V. K. Michaelis, E. Lam, J. Li, A. Moores, *ChemRxiv* **2021** 10.26434/chemrxiv.14541909.v1.

I10 - High entropy alloys: their entropies of mixing and properties

Magdalena Wencka[1,2]
[1]Jozef Stefan Institut, Ljubljana
[2]Institute of Molecular Physics, Polish Academy of Sciences, Poznań
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New approach to metallic alloys design with multiple principal elements in equimolar or near-equimolar ratios, termed high-entropy alloys (HEAs), has been proposed within past decades [1,2]. According to this concept, high entropy of mixing can stabilize disordered solid solution phases with simple structures like a body-centered cubic (bcc), a face-centered cubic (fcc) and a hexagonal close-packed (hcp) with small unit cells, in competition with ordered crystalline intermetallic phases that often contain structurally complex giant unit cells. HEA structure is characterized by a topologically ordered lattice with an exceedingly high chemical (substitutional) disorder, so that a HEA can be conveniently termed as a "*metallic glass on an ordered lattice*". In order to achieve a high entropy of mixing, the alloys must be composed of typically five (or less or more) chemical elements in similar concentrations, ranging from 5 to 35 at. % for each element, but do not contain any element whose concentration exceeds 50 at. %. Physical properties of the HEAs remain largely unexplored. In 2014 the first superconducting HEA within the Ta-Nb-Hf-Zr-Ti system was discovered [3]. HEAs exhibit also rich and complex magnetic field-temperature phase diagrams, including a helical antiferromagnetic structure, a conical structure, a ferromagnetic structure and a spin-glass structure specific to HEA systems. Enhanced mechanical properties like high hardness and solid-solution strengthening are also characteristic to HEAs.

[1] J.W. Yeh et al., *Adv. Eng. Mater*. **6** (2006) 299.
[2] J.W. Yeh, *Ann. Chim. Sci. Mat.* **31** (2006) 633.
[3] P. Koželj et al., *Phys. Rev. Lett.* **113** (2014) 107001.

I11 - Possible superconductivity from carriers that exhibit strange metal behavior in overdoped cuprates

M. Čulo,[1,2] *C. Duffy*,[1] *J. Ayres*,[3] *M. Berben*,[1] *Y.-T. Hsu*,[1] *R. D. H. Hinlopen*,[3] *B. Bernáth*,[1] *N. E. Hussey*[1,3]
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[2]Institute of physics, Bijenička cesta 46, 10000 Zagreb
[3]H. H. Wills Physics Laboratory, University of Bristol, Bristol
e-mail: mculo@ifs.hr

After more than thirty years of intensive research, high-temperature superconductivity in cuprates still remains one of the biggest mysteries in condensed matter physics. Especially interesting is the overdoped part of the phase diagram where superconductivity emerges from a strange metal phase that is no less mysterious. Our recent high-field magnetoresistance study [1] showed that this strange metal phase actually consists of two distinct charge sectors, one governed by standard coherent quasiparticles giving rise to normal metal properties such as the Hall response, and the other governed by incoherent carriers (with no intrinsic Hall response) responsible for strange metal behavior. In addition, the zero-temperature superfluid density exhibits an anomalous depletion with increasing doping while over the same doping range the effective zero-temperature Hall carrier density increases and are both smaller than the total carrier density. Here we present our detailed analysis in overdoped $Tl_2Ba_2CuO_{6+\delta}$ and $La_{2-x}Sr_xCuO_4$ which showed that the growth in the superfluid density, as doping is decreased from the overdoped side, may be compensated by the loss in the coherent carrier density and that their sum is approximately equal to the total carrier density. Such a correspondence, in contrast to the conventional BCS theory, implies that superconductivity in overdoped cuprates emerges uniquely from incoherent carriers that exhibit strange metal behavior.

[1] J. Ayres, M. Berben, M. Čulo, Y.-T. Hsu, E. van Heumen, Y. Huang, J. Zaanen, T. Kondo, T. Takeuchi, J. R. Cooper, C. Putzke, S. Friedemann, A. Carrington, N. E. Hussey, accepted for publication in Nature (2021)
[2] M. Čulo, C. Duffy, J. Ayres, M. Berben, Y.-T. Hsu, R. D. H. Hinlopen, B. Bernáth, N. E. Hussey, submitted to *SciPost. Phys.* (2021)

I12 - Preparation and properties of biomacromolecule@ZIF biocomposites

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A burgeoning research in the field of Metal-organic Framework (MOF) materials is the investigation of porous and dense biocomposites. Biomacromolecules can be integrated with MOFs by surface immobilization, infiltration, and encapsulation.[1,2] This presentation will focus on encapsulation methods via the spontaneous self-assembly of Zeolitic Imidazolate Frameworks (ZIFs) around biomacromolecules (e.g. proteins, enzymes, carbohydrates) and assembly of thereof (e.g. yeast cells).[1,2,3] Recent progress towards the engineering of crystalline phases, particle size and multi-component biocomposites will be disclosed.[4,5,6] The synergy between bio-catalysts, bio-therapeutics, and ZIFs will be examined.
The relevance of these biocomposites for the future progress of MOFs for biotechnology and biomedicine will be illustrated.

[1] M. de J. Velásquez-Hernández, M. Linares-Moreau, E. Astria, F. Carraro, M. Z. Alyami, N. M. Khashab, C. J. Sumby, C. J. Doonan, P. Falcaro, *Coord. Chem. Rev.* **429** (2021) 213651.
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I13 - Living at the edge: Renewable energy relies on meta-stable materials

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Classical materials science may be traced back to the requirements of construction and armor: the harder and the more durable the material, the better. However, the modern challenge of renewable energy is the intermittence and volatility of demand and supply, which is bridged by energy storage and conversion devices. These devices rely on materials, which change their chemical state upon request. Their development and analysis pose new challenges to materials research: the operando investigation of these meta-stable materials. In this talk, I will discuss various examples of energy materials for hydrogen storage [1], heat storage [2], catalysis [3], and electrochemical conversion [4], demonstrating that their development requires more than new analytical techniques, as experimental planning and infrastructure, and even data evaluation is different from the classical investigation of stable materials. The examples highlight that the performance parameters of modern energy materials are rooted in highly dynamic physical processes such as diffusion. It eventually culminates with a new perspective on materials in renewable energy research.

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[2] B. Fumey et al, *Energy Technol*. **8** (2020) 2000187.
[3] J. Terreni, et al., *J. Phys. Chem. C* **122** (2018) 23574 ; J. Terreni et al., *Phys. Chem. Chem. Phys*. **22** (2020) 22979.
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Poster presentations

P01 - Few-body structural properties reveal many-body structures

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By diffusion Monte Carlo and pure estimators [1] we explore [2,3,4,5,6]: ground-state properties of quantum few-body systems, consisting of up to 3 different atomic species; stability and structure of different clusters consisting of spin-polarized H, He, Ne, Ar, alkali and alkaline-earth isotopes; and model systems to test influence of a potential model.

Among structural properties we emphasize helium dimers and trimers which can be compared [6] with the most recent experimental results [7-9] obtained by Coulomb explosion imaging of diffracted clusters, and helium-alkali pentamers [10] which already indicate behavior noticed in nanodroplets [11].

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P02 - Radical Difussion in Glass Forming and Crystallizing liquids

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Diffusion is a random translational motion of molecules and its rate is described by the diffusion coefficient – diffusivity, which is studied by EPR spectroscopy. The diffusion of radicals in a liquid changes the strength of the magnetic interactions between the spins of their unpaired electrons and thus affects the shape of the EPR spectrum of the radicals [1].

By cooling liquids, two different phenomena can occur: crystallization, which is transition from a liquid to a solid state of a high degree of organization [3], and glass transition, which occurs by rapid cooling, formation of a solid amorphous state [2]. We examined the relationship between Tempone diffusivity and self-diffusion coefficients for PC and DMF. These relationships differ (Figure 1) which is possibly due to different cooling behavior and solid structure formation.

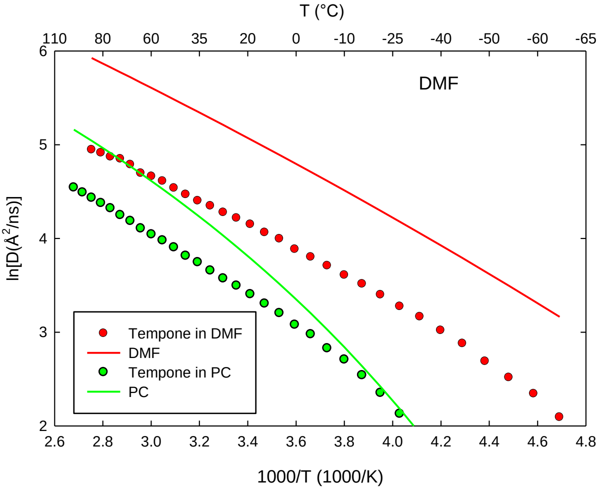

Figure 1 Curves of Tempone diffusivity for PC and DMF.

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P03 - Expanding the crystal form landscape: computational tools for the discovery of eutectics and higher-order cocrystals

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Whilst there have been many reports of the application of computational methods to support the discovery of binary cocrystals, very little is known about the accuracy of computational structure prediction (CSP) methods [1] for supporting the discovery of higher-order cocrystals (HOCs). The discovery of such HOCs widens the crystal form landscape and allows drug developers to choose the optimal solid dosage form for a particular active ingredient. We demonstrate [2] that CSP methods can be adapted to support the discovery of ternary molecular ionic cocrystals comprising many competing hydrogen bonding interactions in the crystal. We also demonstrate that eutectic composite materials with favorable solubility enhancements can be discovered using a weighted Monte Carlo algorithm that computes the mixing energies and binding modes of candidate molecular pairs. Our work demonstrates that computational methods are indispensable in supporting the discovery of new functional crystalline materials of organic compounds.

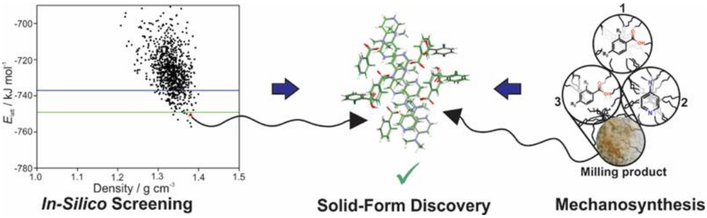

Figure 1 We apply a synergistic mechanochemical milling and *in-silico* screen to discover novel eutectics and higher-order crystals of a range of organic compounds

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P04 - Surface chemistry of ion beam irradiated graphene oxide papers

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Surface chemistry of graphene oxide (GO) plays an important role in possible applications of the material. Beside traditional approaches, like thermal treatment, ion beam irradiation has been recognized as a tool for modifying not only the surface chemistry, but also the structural properties of GO. In this study, the GO paper was irradiated with 15 keV proton beam with fluencies from $5×10^{16}$ to $2×10^{17}$ ions/cm^2. Surface chemistry of GO was monitored with Fourier-transform infrared spectroscopy (ATR-FTIR) and X-ray photoelectron spectroscopy (XPS) while structural changes were investigated with Raman spectroscopy. XPS and ATR-FTIR methods showed partial reduction of GO, with preferential desorption of basal plane alkoxy and epoxy oxygen groups. In terms of structural changes, intensity ratio of D and G peaks decreased linearly with the increase of C/O ratio *i.e.* increase of fluence. The reduction of GO with hydrogen atom was also investigated dynamically by semi-empirical calculations. The calculations for the epoxy group have identified energy ranges at which reduction is a consequence of physical (>20 eV) or chemical (<1.5 eV) processes. The results are showing a potential of ion beam irradiation for controllable modification of structural and surface properties which can be used for tuning of the charge storage properties of graphene oxide.

P05 - Amorphous preformulations of the cucurbit[7]uril inclusion complexes of cyclin-dependent kinase 4/6 inhibitors

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Cucurbit[7]uril (CB[7]) possesses the desired characteristics of a good pharmaceutical excipient. Most importantly CB[7] inclusion complexes can be beneficial for improving the physical stability, solubility, and permeability properties of drugs. [1] Palbociclib (PCB) and ribociclib (RCB) are the cyclin-dependent kinase 4/6 inhibitors (CDK4/6i) [2] having poor water solubility and belongs to BCS classes II and IV drugs, respectively. We had prepared the host-guest complexes of these drugs with CB[7] for their potential application as amorphous solid pre-formulations for addressing the poor water solubility. The formation of the inclusion complexes of both drugs in solution and solid-state was studied from ^{1}H-NMR, UV-Vis, ITC, DSC, and MALDI-TOF analysis. [3] The binding of drugs with CB[7] was assessed with the help of free energy calculations and QTAIM analysis.

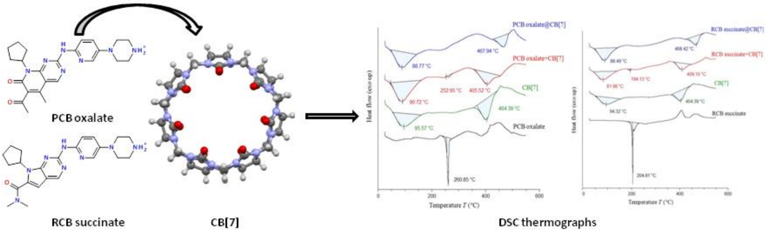

Figure 1 Encapsulation of CDK4/6i within CB[7].

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[2] B. O'Leary, R. S. Finn, N. C. Turner, *Nat. Rev. Clin. Onco.* **13** (2016) 417.
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P06 - Competition of halogen and pnicogen bonds in cocrystals of 2-nitrobenzaldehyde derived imines

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The study of halogen bond in multicomponent systems is one of the most developing areas in crystal engineering and supramolecular chemistry [1]. Alongside the halogen bond, an entire family of related σ-hole interactions, including pnicogen atoms have been described [2]. One of the functional groups that has potential to form both halogen and pnicogen bonds is nitro group [3,4]. In this research, cocrystals of imines derived from 2-nitrobenzaldehyde (**nba**) and 4-X-aniline (**Xan**, X = Cl, Br, I) with 1,3-diiodotetrafluorobenzene (**13tfib**) and 1,3,5-triiodotrifluorobenzene (**135tfib**) were synthesized by cocrystallization from solution and mechanochemically. X-ray structural analysis revealed a successful synthesis of six cocrystals exhibiting 1:1 stoichiometry. In all cocrystals, halogen bond donors and imines are connected *via* $N_{imine}\cdots I$ halogen bonds, while in five cocrystals imines are additionally connected *via* $N_{nitro}\cdots O_{nitro}$ pnicogen bonds, and □□nitro group interactions.

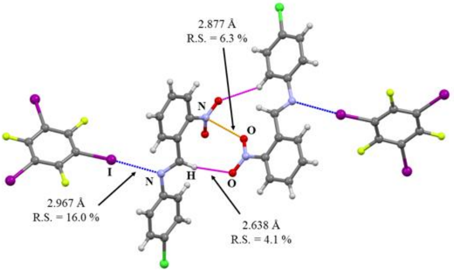

Figure 1 Halogen, pnicogen and hydrogen bonds in (**nbaClan**)(**135tfib**)

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P07- Solvent influence on the crystal packing of supramolecular copper(II) ternary coordination compounds

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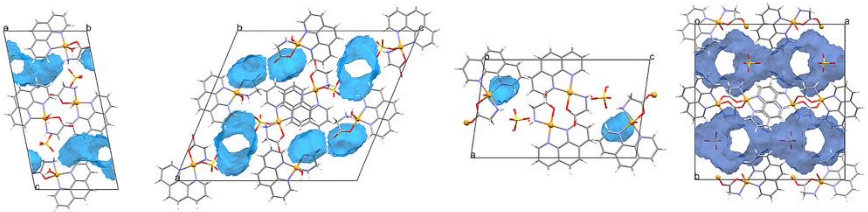
Water adsorption materials have been in focus as potential desiccants or, more recently, as atmospheric water harvesters [1]. Recently we showed that ternary coordination compounds of copper(II), aminoacidates and heterocyclic bases have the potential for controllable water absorption/desorption in the solid state [2]. We report syntheses and crystal structures of ternary coordination compounds of phenanthroline (phen), glycine (HGly) and copper(II): [Cu(Gly)(H$_2$O)(phen)]$_2$SO$_4$·6H$_2$O (**1a·6H$_2$O**), [Cu(Gly)(H$_2$O)(phen)][Cu(Gly)(SO$_4$)(phen)]·5H$_2$O (**1b·5H$_2$O**), {[Cu(μ-Gly)(phen)]$_2$SO$_4$·2H$_2$O}$_n$ (**1c·2H$_2$O**), and {[Cu(μ-Gly)phen)]$_2$SO$_4$·3CH$_3$OH·2H$_2$O}$_n$ (**1c·3CH$_3$OH·2H$_2$O**). Syntheses were performed by solution-based techniques and by liquid assisted grinding. Fine tuning of the synthetic conditions influenced the copper(II) coordination and supramolecular architectures of the compounds. Four types of solvent packing were found: pockets in **1c·2H$_2$O**, 1D channels and pockets in **1b·5H$_2$O**, 1D channels in **1a·6H$_2$O** and 2D channels in **1c·3CH$_3$OH·2H$_2$O** (Figure 1). Stability of compounds under atmosphere of water and methanol vapours was tested.



1a·6H$_2$O 1b·5H$_2$O 1c·2H$_2$O 1c·3CH$_3$OH·2H$_2$O

Figure 1 Four types of solvent packing: 1D channels in **1a·6H$_2$O**, 1D channels and pockets in **1b·5H$_2$O**, pockets in **1c·2H$_2$O** and 2D channels in **1c·3CH$_3$OH·2H$_2$O**.

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P08 - Estimation of the screening of the electron-phonon interaction from ARPES spectra

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In the past years, in numerous angle-resolved photoemission spectroscopy (ARPES) studies [1-3] of a wide class of low-density metallic systems, ranging from doped transition metal oxides to quasi-two-dimensional interfaces between insulators, well separated phonon sidebands below the quasiparticle peak as a unique hallmark of polaronic correlations were observed. However, despite the extensive ARPES data available and numerous works on their first-principle simulations [4,5], little is known about the manifestation of the screening effects on those unique features in ARPES spectra. Thus, we present in this work a methodology to estimate the effective range of the electron-phonon interaction based on the calculation of the leading and next to the leading order in the electron-phonon interaction, including the leading vertex correction, electron self-energy diagrams and the corresponding spectral function. Moreover, we introduce a few estimators related to the confinement of the spectrum intensity within the Fermi surface, which are shown to give a robust estimate of the screening effects regardless of the limited experimental resolution, dimensionality, and particular features of the electronic structure.

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P09 - FTIR analysis of carbonate precursors in manganite coprecipitation synthesis by FTIR spectroscopy

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The simple perovskite oxides, manganites, are nowadays subject of extensive research because of their electrical, magnetic and photocatalytic properties [1-3]. Manganites described with general formula $A_{1-x}Sr_xMnO_3$ (A = Ca, Ba, La) were prepared by the coprecipitation method. Precursors and calcined powders were analyzed by Fourier transform infrared (FTIR) spectroscopy and crystallization was studied by X-ray diffraction. In all systems, successfully doped manganites were obtained by coprecipitation. Positions and shapes of carbonate bands in carbonate precursors FTIR spectra were shown to be useful for screening successful syntheses of doped manganites, particularly in $Ca_{1-x}Sr_xMnO_3$ and $La_{1-x}Sr_xMnO_3$ systems.

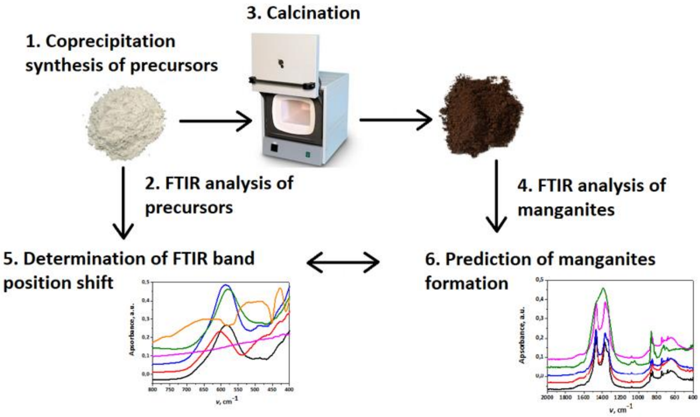

Figure 1 Scheme of experimental procedure

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P10 - Infrared spectroscopic insight into solid-state transformations

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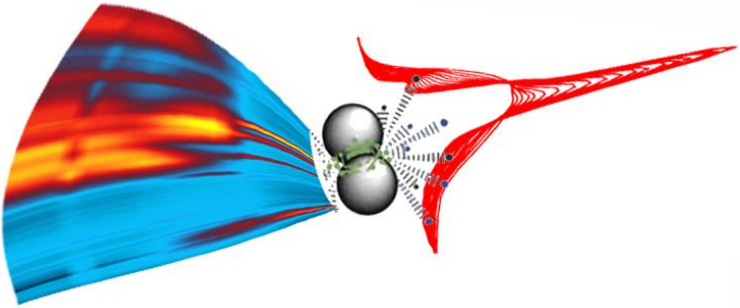
Infrared spectroscopy provides a detailed insight into molecular background of various chemical systems. From the practical point of view, the technique is widespread, not expensive and easy to use. However, it is almost exclusively used just to obtain a basic information on the system under consideration within the materials science community. The purpose of this report is to illustrate the power of this technique on a few examples of solid-state chemical systems, including monitoring of the progress of mechanochemical preparations,[1,2] exfoliations, thermally induced decompositions,[1,3] gas sorption [3] and solid state diffusion-driven processes.[2,4]



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P11 - Cost-effective, high-throughput and high-resolution µRaman spectrometer based on industrial camera

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We have constructed and characterized a µRaman spectrometer that: reaches spatial resolution of <1 µm; is cost-effective; is compact; provides high spectral resolution of 2.6 cm-1 or resolving power of 6400. The key factor to achieve good performances in the latter three parameters has been the design of Raman beam coupling to the entrance slit and the choice of an industrial-grade CMOS camera as detector [1]. The drawback of such type of camera is that integration time is limited to less than 1 s. However, the spectrometer is perfectly suited for confocal Raman imaging where usually <100 ms integration times per spatial point are used. Moreover, by characterization with the 2D MoS_2 sample, we have demonstrated the spectrometer has throughput comparable to research-grade confocal Raman microscopy systems. The reduction of cost by two orders of magnitude compared to research-grade commercial devices will enable an even wider spread of μRaman spectroscopy and strengthen its role in answering fundamental questions in fields of functional materials, mechanochemistry, life and biomedical sciences.

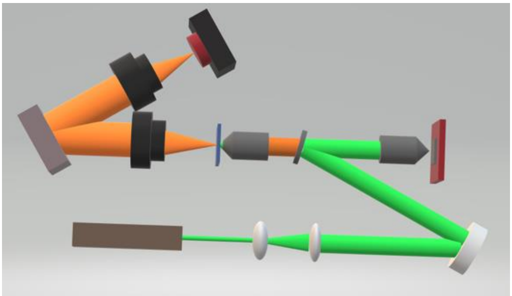

Figure 1 The schematic diagram of the low-cost μRaman spectrometer currently optimized for the 532 nm laser excitation.

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P12 - Mechanochemical synthesis of drug–drug and drug–nutraceutical multicomponent solids of olanzapine

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Drug-drug and drug-nutraceutical cocrystals have immerged as a novel alternative to pharmaceutical cocrystals owing to their importance in reducing drug load and cost effects during multiple disease diagnosis. The major drawback of olanzapine (OLN), an antipsychotic drug is increased blood glucose level along with impotency and weight gain. Here, we synthesized a few drug-drug and drug-nutraceutical multicomponent solids of OLN using mechanochemistry (figure 1). The synthesized OLN–NAT coamorphous salt has a potential scope for development as a combination drug as it reduces blood glucose level, one of the major side-effect of OLN monotherapy. Moreover, the crystalline salt of OLN–PZO can be used as a combination drug for TB patients with bipolar disorder.[1]

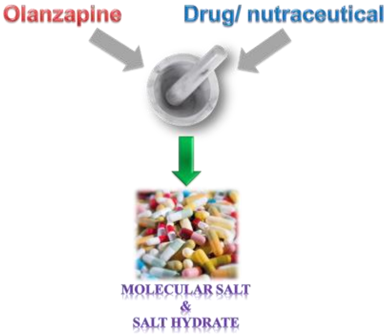

Figure 1 Drug-drug and drug-nutraceutical multicomponent solids prepared using mechanochemistry.

[1] K. K. Sarmah, N. Nath, D. R. Rao. R. Thakuria, *CrystEngComm.* **22** (2020) 1120.

P13 - One-Step Mechanosynthesis of Graphene Quantum Dots

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Graphene quantum dots (GQDs) have attracted significant attention due to its intriguing physicochemical properties which makes it a good material for potential applications in bioimaging, sensing, solar cells, photovoltaic devices, photocatalysis and white-light-emitting diodes [1]. Nevertheless, industrial GQDs synthesis is strenuous due to the toxicity and longevity of thus far invented processes [2]. Therefore, a facile and highly reproducible approach for the large-scale generation of GQDs with minimal surface defects is required. Herein we describe environmental-friendly, solid-state mechanosynthesis of GQDs.

[1] V. Georgakilas, J. A. Perman, J. Tucek R. Zboril, *Chem. Rev.* **115** (2015) 4744
[2] Z. Zhipan, Z. Jing, C. Nan, Q. Liangti, *Energy Environ. Sci.* **5** (2012) 8869

ACKNOWLEDGMENTS

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P14 - Mechanochemical synthesis and characterisation of Pt-SnO_2 and Pt-Fe_2O_3 nanomaterials

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Nanocrystalline samples of hematite (α-Fe_2O_3) and cassiterite (SnO_2) were synthesized by activating Fe (II) acetate and Sn (II) acetate in a planetary mill followed by heat treatment to 600 °C. The XRD results showed that the hematite sample possessed a volume average crystal domain size of 26 nm, and the upper limit of microstrain was 1×10^{-4}. The average size of the cassiterite crystal domain is 29 nm. The Williamson-Hall analysis of the cassiterite showed the presence of anisotropy, with slightly narrower diffraction lines with Miller indices hk2, indicating an increase in the size of the crystal domain (the values in the hk2 direction were estimated to be 34 nm). Hematite and cassiterite samples were doped with platinum in three ways, *(i)* in one step by mixing powdered Fe (II) acetate or Sn (II) acetate precursor with Pt $(Acac)_2$ and activation in a planetary mill followed by annealing at 600 °C, *(ii)* in two steps, where first hematite (α-Fe_2O_3) and cassiterite (SnO_2) were synthesized at 600 °C and then the pristine powder samples were mixed with Pt $(Acac)_2$ precursor and homogenized by grinding for 2 h in a planetary mill. Then the homogenized samples were annealed to 400 °C, *(iii)* the samples were synthesized in two steps, with the difference that a certain amount of Pt $(Acac)_2$ was dissolved in toluene and then mixed and homogenized with Fe (II) acetate or Sn (II) acetate precursors, and then the samples were homogenized in a planetary mill and annealed to 400 °C. Platinum (Pt) in the samples was detected directly by EDS analysis and indirectly by TPR (Temperature Programmed Reduction in hydrogen) results.

P15 - Mechanochemical activation of $LiAlH_4$-Fe_2O_3 composites-a method to enhance kinetics of hydrogen desorption

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Mechanical milling of pure lithium alanate ($LiAlH_4$) was done with addition of 5 weigh percent of Fe_2O_3 using different milling time ranging from 1 to 15 minutes [1]. Mechanical milling of composites causes destabilization of $LiAlH_4$ structure as it observed by XRD measurements. Particle size distribution results reveals that composite particle size decrease with milling time up to 3 minutes, and then increase almost to the original size, for 15 min sample. Mechanical mailing cause phase transformation from AlH_4^- to AlH_6^{3-}. As a consequence of structural and chemical changes, desorption properties of composites are change kinetic of desorption is improved in comparison to unmilled $LiAlH_4$. The shifting of hydrogen desorption temperature to lower temperatures is observed together with change from multi-step desorption to one-step hydrogen desorption is also observed. This caused decrease in activation energy of composites from E_a = 665 kJ/mol for unmilled $LiAlH_4$, E_a = 279 kJ/mol for 3 min milled composite.

[1] M.Dragojlović, I.Milanović , A.Gradišek, S.Kurko, M.Mitrić, A.Umićević, J.Radaković, K.Batalović, *Int. J. Hydrog. Energy* **46** (2013) 13070.

P16 - Mechanochemical Synthesis of Novel Mg- and Ca-Containing Bimetallic Amidoboranes

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Mechanochemistry can be very useful for synthesis of bimetallic amidoboranes - very prominent materials for hydrogen storage. By using the mechanical ball milling technique, solventless solid state reaction between ammonia borane (NH3BH3), alkali metal hydrides (NaH, LiH) and alkaline earth metal hydrides (CaH_2 and MgH_2) is absolutely possible [1,2]. Exclusively hydrogen and bimetallic amidoboranes are obtained as final products. Here we report several examples of successful synthesis - $Na_2Mg(NH_2BH_3)_4$, $Li_2Mg(NH_2BH_3)_4$, $Na_2Ca(NH_2BH_3)_4$ and $Li_2Ca(NH_2BH_3)_4$ – all prepared and characterised by our group.

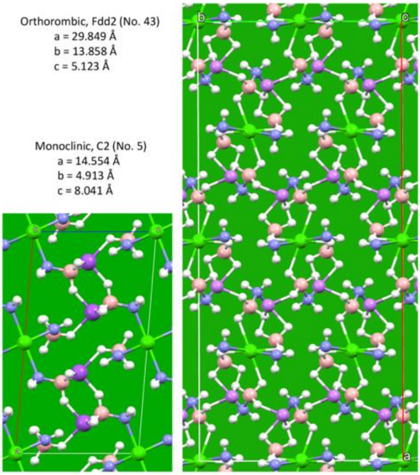

Figure 1 Unit cells of synthesized Ca-containing amidoboranes. Left) $Na_2Ca(NH_2BH_3)_4$; Right) $Li_2Ca(NH_2BH_3)_4$.

[1] I. Milanović et al., *ACS Sus. Chem. Eng.* **9** (2021) 2089.
[2] N. Biliškov et al., *Chem. Eur. J.* **23** (2017) 16274.

P17 - Mechanochemical metathesis and double salt formation

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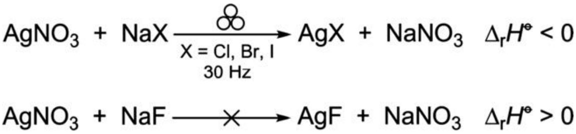
Mechanochemical milling was successfully applied to prototypical metathesis reaction between $AgNO_3$ and NaX (X = Cl, Br, I) [1]. This approach also successfully demonstrated the synthetic path to Ag_2XNO_3 double salts. Real-time and in situ reaction monitoring using synchrotron powder X-ray diffraction (PXRD) and Raman spectroscopy revealed that only in the case with NaBr metathesis reaction underwent without the formation of intermediate phases. With NaCl, the Ag_2ClNO_3 appeared as the intermediate, while with NaI, a short-living intermediate phase was observed in PXRD (on average living for 30 seconds) and could not be fully characterized. As expected from standard reaction Gibbs energies of reactants and products, milling with NaF gave the mixture of starting materials. In comparison to performing this reaction in solution, where it is driven by the extremely low solubility of silver products and their immediate precipitation, in the solid state, reactions proceed through the formation of reactive intermediates and provide an elegant way of preparing corresponding double salts.



$$AgNO_3 + NaX \xrightarrow[\text{X = Cl, Br, I; 30 Hz}]{} AgX + NaNO_3 \quad \Delta_r H^\circ < 0$$

$$AgNO_3 + NaF \not\rightarrow AgF + NaNO_3 \quad \Delta_r H^\circ > 0$$

Figure 1 Ion metathesis reactions between $AgNO_3$ and NaX (X = Cl, Br, I).

[1] S. Lukin, T. Stolar, I. Lončarić, I. Milanović, N. Biliškov, M. di Michiel, T. Friščić, I. Halasz *Inorg. Chem.* **59** (2020) 12200.

P18 - Competitive cocrystallization reactions in the solid state

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Mechanochemical milling is an efficient method for solid-state preparation of cocrystals. However, when more than one cocrystal is present in the solid mixture of several potential coformers, competitive reactions could take place [1]. Here, we present the study of competitive cocrystallizations for cocrystals of urea and ortho- (o-OH-Ba), meta- (m-OH-Ba), and para-hydroxybenzoic acids (p-OH-Ba), each of which forms different stoichiometric cocrystal with urea (Figure 1). From neat and liquid-assisted grinding experiments, we derived the relative thermodynamical stabilities of cocrystals to be m-OH-Ba < o-OH-Ba< p-OH-Ba. Reaction profiles derived from in situ Raman monitoring for cases when only one or more cocrystals can form revealed that the rate of formation of the most stable cocrystal, p-OH-Ba:urea is increased regardless of the presence of competitive coformer. Interestingly, its formation was the slowest in experiments comparing the formation of cocrystals without competing coformer.

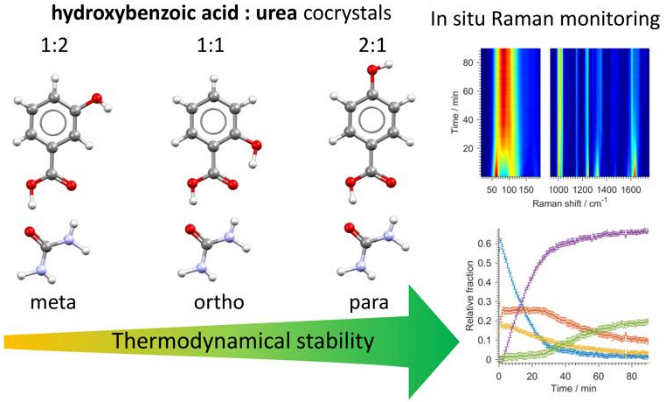

Figure 1 Competitive cocrystallization in a ball mill.

[1] S. Lukin, I. Lončarić, M. Tireli, T. Stolar, M. V. Blanco, P. Lazić, K. Užarević, I. Halasz, *Cryst. Growth Des.* **18** (2018) 1539.

P19 - Mechanochemical synthesis of value-added fertilizer from low-cost starting materials: exploring the reaction space

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Urea is an easily available and effective nitrogen fertilizer, that suffers from decomposition issues, resulting in watershed and air contaminants, as well as decreased absorption by plants. One way of tackling this problem is the formation of urea adducts, such as tetrakis(urea) calcium sulfate (**1**) that can provide other essential plant nutrients, and stabilize urea in the soil. [1]

We explore here the mechanochemical synthesis of **1** [2] from urea and gypsum derivatives (gypsum, calcium sulfate hemihydrate, anhydrous calcium sulfate). We compare different synthetic methods (ball mill, planetary mill, twin screw extruder) at different temperatures, and monitor the reaction kinetics by Raman spectroscopy and synchrotron X-Ray Diffraction.

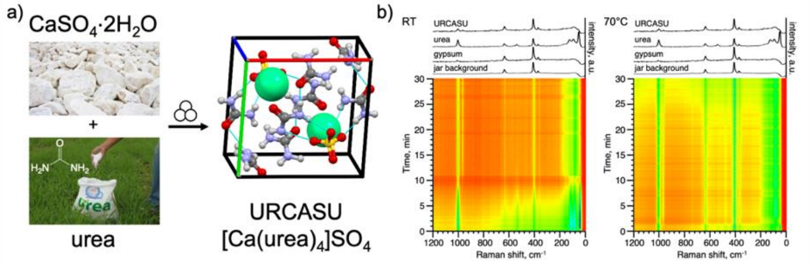

Figure 1 a) Schematic representation of the mechanochemical synthesis of **1**. b) Raman monitoring of neat grinding synthesis of **1** at room temperature (left) and 70°C (right).

[1] J. P. R. de Villiers, J. C. A. Boeyens, *J. Cryst. Mol. Struct.* **5** (1975) 215.

[2] K. Barčauskaitė, Z. Brazienė, D. Avižienytė, M. Silva, D. Drapanauskaite, K. Honer, K. Gvildienė, R. Slinksiene, K. Jancaitiene, R. Mazeika, G. Staugaitis, T. Dambrauskas, K. Baltakys, J. Baltrusaitis *J. Env. Chem. Eng.* **8** (2020) 103965.

P20 - Electrochemical Detection of Arsenic^{3+} on Gold α-$K_{015}MnO_2$, α-$K_{018}MnO_2$ and β-MnO_2 Electrodes

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About one hundred million people around the world are being exposed to water polluted by toxic arsenic where prolonged exposure to arsenic has a detrimental effect on human health. Consequently, the World Health Organization has limited the maximum level of arsenic in drinking water to 10 μg L^{-1}[1]. In this work, three MnO_2 electrodes, synthesized by the hydrothermal procedure as in ref. [2], and then coated with gold, were tested for As^{3+} sensing in acidic media (0.5M H_2SO_4) by anodic stripping voltammetry. Voltammograms of all three materials showed a well-defined peak at ca. 0.25 V vs SCE corresponding to the electrooxidation of As, but the lowest limit of detection of 1.34 ppb was obtained using the Au/β-MnO_2 electrode. Also, the possibility of using these electrodes for the detection of As^{3+} in real samples was tested in water sample from river Drina and tap water. The responses of the electrodes in real samples (without any prior treatment) were well defined by the appearance of a clear peak corresponding to As^{3+} oxidation.

[1]X. Xu, X. Niu, X. Li, Z. Li, D. Du, Y. Lin, *Sens. Actuators B Chem* **315** (2020) 128100.
[2]Z. Li, Y. Ding, Y. Xiong, Y. Xie, *Cryst. Growth Des*. **5** (2005) 1953.

P21 - Hyperthermic potential of magnetic iron oxide nanoparticles prepared by oxidation-precipitation

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Four samples containing magnetic iron oxide nanoparticles (MIONs) were prepared using a simple oxidation-precipitation method from iron(II) salt solution, in the presence of NaNO3 as an oxidant. Preparation of two samples also involved use of the chelating agent ethylenediaminetetraacetic acid (EDTA). Depending on the molar ratio of the reactants used, MIONs samples having average particle size between 7 nm and 32 nm were obtained, as revealed by TEM imaging. X-ray diffraction study shows that all samples crystallized in the cubic spinel structure (S.G. *Fd*3*m*), with average crystallite size in the range of 6 to 26 nm. Bigger MIONs (MAG29 and MAG32), with broaden size distribution, and composition close to magnetite, form big aggregates in aqueous suspension (d_{hyd}~600 nm), while the size of aggregates of 7nm- and 14nm-sized MIONs is significantly lower. Potential biomedical application of the samples suspended in water was evaluated by studying magnetic and hyperthermic properties. Samples containing smaller nanoparticles, with higher volume fraction of superparamagnetic particles at room temperature, showed better magnetic heating ability.

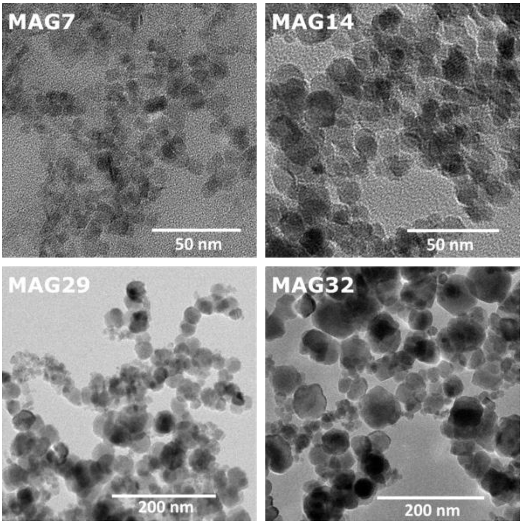

Figure 1 TEM micrographs of the synthesized MIONs. The samples were named according to the average particle sizes.

P22 - Magnetic properties of composite poly(ethylene oxide)/iron oxide hydrogels

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Magnetic polymer gels (ferrogels) are a new promising class of nanocomposite hydrogels, with potential application in soft actuators such as artificial muscles, in tissue engineering, drug delivery and hyperthermia applications. Although γ-irradiation method is highly suitable for generation of nanoparticles (NPs) in a solution as well as for the formation of three-dimensional polymer network, i.e. hydrogels, the radiolytic syntheses of iron oxide/polymer nanocomposite gels are rarely investigated, especially in the case of one-step synthetic approaches, such as the one used in this work. The radiolytic one-step synthesis resulted in the simultaneous crosslinking of the PEO polymer and the reduction of iron (III) salt (Figure 1). Electron microscopy, XRD, SQUID and Mössbauer measurements identified the particles as magnetite/maghemite and showed that they were < 5 nm in size, superparamagnetic and that there was a significant contribution of surface effects on the magnetic properties of the nanoparticles embedded in the hydrogel [1].

Acknowledgments: This work has been supported by the Croatian Science Foundation under the project UIP-2017-05-7337 (POLRADNANOP).

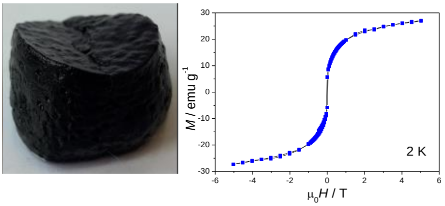

Figure 1. A photograph of a composite hydrogel (left) and its magnetization behavior at 2 K (right)

[1] I. Marić, N. Šijaković-Vujičić, A. Pustak, M. Gotić, G. Štefanić, J.-M. Grenèche, G. Dražić, T. Jurkin, *Nanomaterials* **10** (2020) 1823.

P23 - Electrical transport and magnetic dynamics in M-type hexaferrites

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Hexaferrites are a class of iron compounds which crystalize in a sandwich-like periodic stacking of iron-oxide layers containing different metal atoms. The simplest is the M-type with chemical formula $AB_{12}O_{19}$, where A = Ba, Pb … and B = Fe, Ti … [1]

Our recent research [2,4] on various substitutions within the M-type hexaferrite has shown signatures of exotic phenomena which point toward a general relaxational mechanism in ferrimagnetic semiconductors. Frequency-dependent magnetic susceptibility (Fig. 1) and dc electric transport properties of three different compositions of hexaferrite $Ba_{1-x}Pb_xFe_{12-y}Al_yO_{19}$ show a correlation between activation energies which persists in the whole researched range of aluminum substitution x = 0 to 3.3. This result is discussed in the context of charged magnetic domain walls, the pinning of which is determined by charge carriers activated over the transport gap.

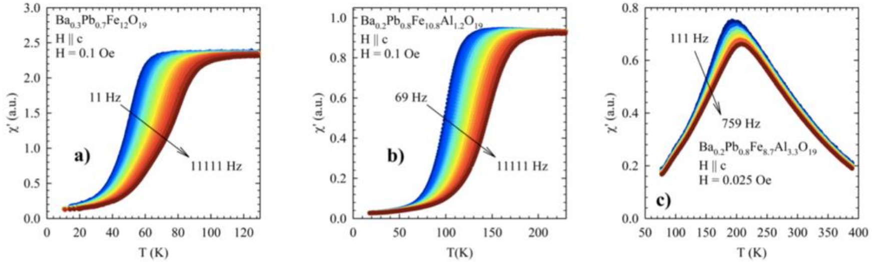

Figure 1. Real part of AC susceptibility for different compositions of $(Ba,Pb)(Fe,Al)O_{19}$ M-type hexaferrites as a function of temperature and frequency.

[1]R. C. Pullar, Prog. Mater. Sci **57** (2012) 1191.
[2]L. N. Alyabyeva et al., New J. Phys. **21** (2019) 063016.
[3]Ž. Rapljenović et al., Persisting correlation between electrical transport and magnetic dynamics in M-type hexaferrites, unpublished results (**2021**).

P24 - Effects of morphology on electrochemical performance of mechanochemically milled molybdenum disulfide

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Mechanochemical modification of the material using ball milling is an extremely suitable method for material modification that can induce a decrease in particle size and crystallite, but also an increase in the microstrain of the crystal lattice [1]. During mechanical milling, the specific surface area of the material and the number of available catalytically active edges in the material increase, which results in improved electrochemical performances. In addition, various additives can be introduced to material that can enhance the properties of the material and obtain composites of the desired characteristics. On the other side, via hydrothermal synthesis, as another easygoing process, the morphology of material can be very efficiently modified and materials of the desired shapes and sizes can be obtained. Additionally, hydrothermal pretreatment improves effects of milling by inducing better delamination of layers [2].

Therefore, molybdenum disulfide was synthesized hydrothermally and after that was milled using high-energy ball mill SPEX Mixer/Mill 5100. The influence of different milling times on the morphology and electrochemical properties of the material is investigated.

[1] S. Kurko et al., *Int. J. Hydrog. Energy*, **38** (2013) 12140.
[2] M. Ahmadi, et al. *Nanomaterials*, **9** (2019) 1400.

P25 - Low temperature electrical characterization of WN_x

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Today, transition metal nitrides are of interest both because of their good electrical properties, which make them candidates for new electrode materials, and because of their mechanical properties, which make them suitable for the design of new cutting tools [1][2].

We report low temperature electrical properties (resistivity, thermopower and magnetoresistance) of WN_x pelet, where x is the yet unknown nitride to metal ratio. From about 20 K to 300 K, the resistance shows a clear Mott-like temperature behaviour (proportional to T^(-1/4)), while below 20 K, the resistance is proportional to T^(-2/5). In <20 K regime we also observe nonlinearities in the Seebeck effect, which suggests a change of dominant conducting mechanism.

Magnetoresistance is measured in a magnetic field directed both parallel and perpendicular to the sample plane. In both cases, the magnetoresistance curves have a similar shape with pronounced local minima at magnetic fields of about 5 T.

[1] Y. Zhou, W. Guo, T. Li, *Ceram. Int.* **45** (2019) 21062.
[2] F. Kawamura, H. Yusa, T. Taniguchi, *J Am Ceram Soc.* **101** (2018) 949.

P26 - Electrical and magnetic features of a 3D oxalate-bridged [CuFe] molecular precursor

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Due to the rich variety of metal species and ligands, coordination geometry, guests inside the pores, and supramolecular structures, an enormous number of coordination polymers with various structures, dimensionality, and nuclearity have been synthesized and reported. This area of molecular chemistry is the basis for design of the molecule-based materials that combine two (or more) physical properties of interest, especially upgrading and expanding the molecular magnetism toward multifunctional systems. Most of the oxalate-based molecular magnets described to date have been obtained by the "complex-as-ligand approach"; a molecular building block, the tris(oxalato)metalate $[M^{III}(C_2O_4)_3]^{3-}$ anion is used as a ligand toward other metal cations. The topology of these oxalate-bridged compounds is controlled by a templating counterion.

Two polymorphs of 3D coordination polymer $[Cu^{II}Fe^{II}_2(H_2O)(terpy)(C_2O_4)_3]_n$ (**1**; terpy = 2,2′:6′,2′′-terpyridine), formed hydrothermally, contain homometallic 2D oxalate-bridged honeycomb anionic layers, $[Fe^{II}_2(C_2O_4)_3]_n^{2n-}$, mutually linked by complex cations of copper(II) ions, $[Cu(H_2O)(terpy)]^{2+}$, through oxygen atoms from oxalate bridges. Recently published oxalate-based networks have shown proton conductivity related to the presence of ammonium and/or crystallization water [1]. Therefore, in addition to magnetic, electrical properties of **1** have been also investigated; it exhibits antiferromagnetic phase transition at 25 K and proton conductivity.

Furthermore, the ability of this 3D polymer, due to their appropriate stoichiometry of metal ions, to act as single-source precursor for the formation of spinel $CuFe_2O_4$ oxide by heat treatment has been explored [2].

[1]L. Kanižaj, D. Barišić, F. Torić, D.Pajić, Krešimir Molčanov, Ana Šntić, I. Lončarić, M. Jurić, *Inorg. Chem.* **59** (2020) 18078.

[2]L. Androš Dubraja, D. Pajić, M. Vrankić, J. Dragović, M. Valant, M. Benčina, M. Jurić, *J. Am. Ceram. Soc.* **102** (2019) 6697.

P27 - Bis(oxalato)chromium(III) complexes with azabicyclic cations: structural and dielectric studies

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Ferroelectric materials exhibit spontaneous electric polarization that can be reversibly switched under external applied electric field. In recent years, ferroelectrics have been extensively investigated, showing promising applications in various microelectronic devices.[1] In attempt to design new molecular ferroelectric crystals, two metal-organic complex salts containing bicyclic amine cations, O-ABCO$^+$ (1-azabicyclo[2.2.2]octan-3-one) and COOH-OH-ABCO$^+$ (3-hydroxy-1-azabicyclo[2.2.2]octane-3-carboxylic acid), and bis(oxalato)chromium(III) anions, $[Cr(bpy)(C_2O_4)_2]^-$ (bpy = 2,2′-bipyridine), were prepared using mechanochemical synthesis. Single crystals of prepared complex salts were obtained by slow evaporation of their aqueous solutions, which allowed structure determination from single-crystal X-ray diffraction analysis. Thermal analysis showed that water molecules of crystallization are retained in the structure up to 100°C. Temperature dependent dielectric studies were performed in -90–100°C temperature range. For compound $(O\text{-}ABCO)[Cr(bpy)(C_2O_4)_2]\cdot H_2O$ dielectric constant and loss increase while increasing the temperature and decrease toward higher frequencies, pointing to its semiconducting nature. Polarization–voltage measurements were conducted to further study the observed dielectric anomalies in this sample.

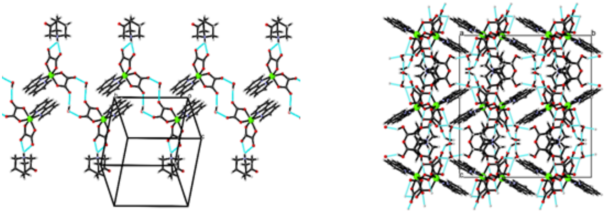

Figure 1 Hydrogen bonding and aromatic stacking interactions in $(O\text{-}ABCO)[Cr(bpy)(C_2O_4)_2]$ (left) and $(COOH\text{-}OH\text{-}ABCO)[Cr(bpy)(C_2O_4)_2]$ (right).

[1] Y.-L. Liu, J.-Z. Ge, Z.-X. Wang, R.-G. Xiong, *Inorg. Chem. Front.* **7** (2020) 128.

P28 - Continuous-wave EPR study of MOF-525 and PCN-223 doped with copper(II) ion as the metal center

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The magnetic properties of metal-organic frameworks MOF-525 and PCN-223 doped with copper (II) ions were examined by continuous wave (CW) EPR spectroscopy. MOF-525 and PCN-223 have different topologies: MOF-525 cuboctahedron and PCN-223 hexagonal prism. [1] Simulations of experimental spectra were done assuming axial symmetry of **g**- and **A**- hyperfine tensors while all four nitrogens in the porphyrin ring were assumed equivalent. The following copper electron spin (S = 1/2) interactions with the nuclear spins were considered: hyperfine interaction with the copper nucleus spin (I_{Cu} = 3/2) and superhyperfine interaction with four neighbouring nitrogen nuclei spins (I_{N} = 1). [2] Fullerene was incorporated to PCN-223 in order to study its influence to spintronic properties. From the simulations of the experimental data we can see that the CW-EPR spectra of MOF-525 and PCN-223 exhibit different hyperfine tensors, that superhyperfine lines are more pronounced if copper ions are more diluted and that fullerene is incorporated into the structure of PCN-223. Simulations were obtained using EasySpin software [3] and one of the representative spectra is shown in Figure 1.

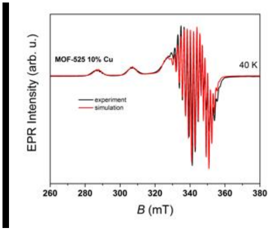

Figure 1 Experimental and simulated CW EPR spectrum recorded at 40 K of MOF-525 with 10% Cu (molar percent).

[1] B.Karadeniz et al., *J. Am. Chem. Soc.* **141** 49 (2019) 19214.
[2] C.Finazzo et al., *Phys. Chem. Chem. Phys.* **8** (2006) 1942.
[3] S. Stoll, A. Schweiger, *J. Magn. Reson.***178** (2006) 42.

P29 - Magnetic properties of mixed copper/zinc MOF-74 compounds and their amorphous phases

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Y. Krupskaya,[3] *V. Kataev*[3]
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Here we present the results of the study of magnetic properties of copper(II)-MOF-74 materials (Cu-MOF-74) and their three mixed analogues with zinc(II). CuZn-MOF-74 and ZnCu-MOF-74 were obtained through different intermediate complexes, namely from magnetically also interesting Cu-INT or from non-magnetic Zn-INT, respectively. The alloyed Cu-MOF-74-Zn-MOF-74 was obtained by growing the MOF structure from the mixture of milled Cu-MOF-74 and Zn-MOF-74 exposed to solvent vapors (accelerated ageing).[1] Additionally, we investigated how the amorphization process influences the magnetic properties of studied crystalline copper/zinc MOF-74 compounds.[2] Magnetic characterization was obtained by static magnetization measurements, X-band electron spin resonance (ESR) spectroscopy as well as multifrequency high-field high-frequency ESR (HF-ESR) spectroscopy.

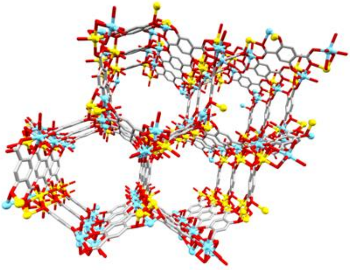

Figure 1 Copper(II)/zinc(II) MOF-74 structure.

[1] G. Ayoub et al, *Chem. Mater.* **31** (2019) 5494.
[2] S. Muratović et al, *J. Mater. Chem. C* **8** (2019) 7132.

P30 - Tuning Magnetism in Mn-doped $CH_3NH_3PbI_3$ perovskites

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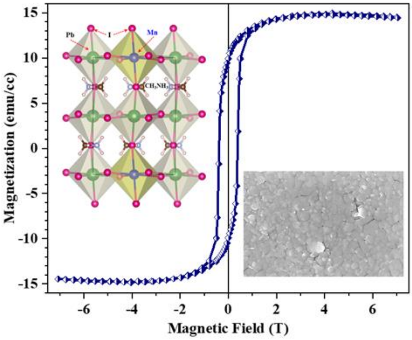
In recent years perovskite halide compounds have attracted numerous attentions for the fabrication of highly efficient solar cells, light emitting diodes, X-ray detection. However, a comprehensive understanding of its microscopic origins has not been fully explored. In this work, the effect of Mn doping in organic-inorganic perovskite semiconductor methylammonium lead iodide ($CH_3NH_3PbI_3$) has been studied. The occurrence of magnetism in $CH_3NH_3PbI_3$ ($MAPbI_3$) has been confirmed from magnetization measurements. The influence of Mn doping in $MAPbI_3$ films, structural and morphological has been analyzed in details. Room temperature ferromagnetism is achieved by incorporation of Mn^{2+}/Mn^{3+} ions into Mn (3-20%) doped $MAPbI_3$ films. Drastic enhancement of magnetic moment is obtained in the Mn (15%) doped $MAPbI_3$ by the effect of eminent double exchange and super exchange interactions in between the Mn^{2+}-I^--Mn^{3+} ions compared with other doping concentration. The investigation of such a drastic enhancement of the magnetic moment has been discussed in detail. Our finding offers an alternative pathway for spintronic, light controlled magnetic and photovoltaic devices.



[1] L. Ren *et al.*, *J. Phys. Chem. Lett.* **11** (2020) 2577.
[2] B. Náfrádi *et al.*, *Nature Commun.* **7** (2016) 1.

P31 - Stabilizaton of FAPI perovskite on ZnO nanorods

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Organometal lead hailde perovskite materials have shown promising properties as active layers for their use in photovoltaic devices [1]. The issue of stability in ambient enviroments still remains a challenge of perovskite thin films due to the degradation when in contact with water molecules [2]. One of the proposed additives for the stabilization of perovskite thin films is polyvinylpyrrolidone [3]. In this work we have studied polyvinylpyrrolidone mixtures with $FAPbI_3$ perovskites and the influence of the polymer on structural stability, morphology and optical propeties of perovskite thin films on nanostructured ZnO thin films.

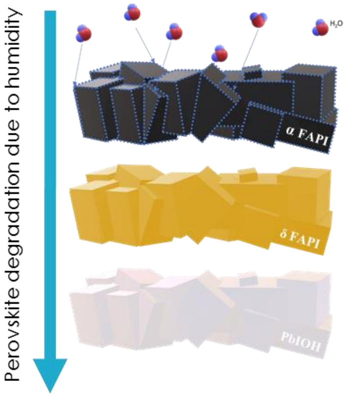

Figure 1 $FAPbI_3$ degradation under the influence of air moist

[1] Kojima, A. et al., *J. Am. Chem. Soc.* **131** (2009) 6050
[2] Niu, G. et al., *J. Mater. Chem.* **2** (2015) 8970
[3] Yan, J. et al., *Sustain. Energy Fuels* **3** (2019) 3448

ERDF (IRI) project "Improvement of solar cells and modules through research and development" (KK.01.2.1.01.0115
This work has been supported by Croatian Science Foundation, IP-2018-01-5246

P32 - Advanced photocatalytic properties of ZnO prepared by thermal decomposition of the cellulose template

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One of the innovative methods of water purification from organic pollutants is based on the photocatalytic ability of semiconductors such as zinc oxide (ZnO) [1]. With this study we will present photocatalytic properties of hybrid materials based on: a) cellulose and zinc oxide (ZnO), and b) ZnO structures obtained by thermal decomposition of the previously prepared ZnO/cellulose hybrids. We synthesized ZnO on two different cellulose substrates, Sodra Green T and UPM Conifer, using the plasma-enhanced atomic layer deposition (PE-ALD) method. After synthesis, the hybrid materials were calcinated in the furnace to obtain pure ZnO. We used field emission scanning electron microscope (FE-SEM) and X-ray photoelectron spectroscopy (XPS) for the characterization of the given samples. Methyl orange (MO) was used, as an organic dye, to examine the photocatalytic properties of the samples. FE-SEM images revealed that calcinated samples have porous tubular structures that are characterized by large specific surfaces. XPS spectra showed that ZnO which was synthesized on Sodra Green T cellulose has a larger amount of reactive OH groups indicating better photocatalytic activity. After calcination of the hybrid materials, ZnO showed enhanced photocatalytic properties. Within 80 min there is complete mineralization and decolorization of MO solution. Furthermore, ZnO deposited on Sodra Green T cellulose substrate proved to be a better photocatalyst than ZnO deposited on UPM Conifer cellulose substrate.

[1] C. Nie, J. Dong, P. Sun, C. Yan, H. Wu, B. Wang, RSC Adv. **7** (2017) 36246.

P33 - GNN and transfer learning for prediction of formation enthalpy of metal hydrides

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Prediction of metal hydride formation enthalpy is one of the key elements for a rapid screening and design of new hydrogen storage materials. In the last decades, DFT (density functional theory) approach showed good predictive potential for the ground state properties and calculation of hydride formation energies. Recently, graph neural network (GNN) implementations show promising results for fast and reliable prediction of formation energies for molecules and crystals. Here, we consider approach for universal machine learning based on a MatErials Graph Network (MEGNet) [1] that enable hydride formation energy prediction with a DFT accuracy. We demonstrate wide screening of potential dopants in Mg_2FeH_6 and Mg_2NiH_4. In addition, we study the potential of transfer learning for building the universal machine-learning model capable of addressing experimentally reported hydride formation enthalpies.

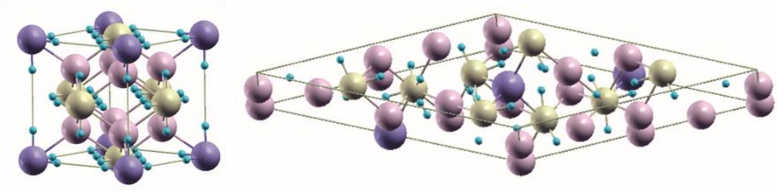

Figure 1 Unit cells of the doped Mg_2FeH_6 (left) and Mg_2NiH_4 (right)

[1] C.Chen, W.Ye, Y.Zuo, C.Zheng, S.P.Ong, *Chem. Mater.* **31** (2019) 3564.

P34 - Hydrogen spillover in hydrogenation catalysts by neutron imaging

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Hydrogenation reactions are crucial in a renewable energy scenario, notably to facilitate the production of hydrocarbons from hydrogen. The reactions are catalyzed by specific catalysts consisting of metal nano-particles on an oxide support, which functions is known to be more than that of a support [1]. Hydrogen after dissociative chemisorption may migrate over the oxide surface and thereby promote the transport to and from the reactive sites [2]. Verification of this so-called hydrogen spillover and particular its effect on the reaction kinetic is an analytical challenge because the quantitative detection of dynamic hydrogen at relatively low concentrations ($c_H \ll 1$ at.%) is difficult. We developed a combinatorial setup for neutron imaging, capable of measuring up to 69 samples simultaneously under identical conditions (temperature/pressure) to quantify the amount of hydrogen in different methane and methanol catalysts.

Hydrogen/deuterium exchange measurements at temperatures between 20 to 300°C and at a pressure of 1bar were performed on Ni deposited on reducible and non-reducible supports. Hydrogen spillover on the Al_2O_3 support proceeds via natural hydroxy groups on its surface in contrast to TiO_2 and SiO_2. Here, spillover is observed only at sufficiently high water partial pressure.

[1] S. J. Tauster, et al., Science **211** (1981) 1121.
[2] W. Karim, et al., Nature **541** (2017) 68 ; R. Prins, *Chem. Rev*. **112** (2012) 2714.

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P35 - Improvement of Hydrogen Storage Properties of MgH_2 by $NaNH_2$ addition

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N. Novaković,[1] *A. Mitrović,*[1] *J. Grbović Novaković*[1]
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MgH_2 based composites with addition of $NaNH_2$ (2 and 5 wt.%) as dopant were synthesized by mechanical milling using three different milling times. The hydrogen desorption properties and kinetic of these composites were examined using Thermal Desorption Spectroscopy (TDS), X-Ray Diffraction (XRD) for microstructure and particle size information and laser scattering method for estimation of particle size distribution (PSD) [1]. Samples with 5 wt.% of dopant and milling time of 15 and 30 minutes shows hydrogen desorption peaks shifting to lower temperatures in contrast to milled and as received MgH_2. All investigated composite samples shows enhanced kinetics with lowered E_a. Different Avrami parameter values were obtained for $NaNH_2$-MgH_2 composites and for pure MgH_2. With the milling time increasement (30 and 60 minutes) of the $NaNH_2$-MgH_2 composites, catalytic activity of $NaNH_2$ decreases which is followed by hydrogen desorption peaks shifting to higher temperatures.

[1] I. Milanović, S. Milošević, Lj. Matović, R. Vujasin, N. Novaković, R. Checchetto, J. Grbović Novaković, *Int. J. Hydrog. Energy* **38** (2013) 12152.

P36 - Modelling of perovskite solar cell

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[3]Ruđer Bošković Institute, Zagreb
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Since their discovery in 2009 [1], perovskite solar cells (PSC) have drawn great attention. The use of methylammonium lead triiodide (MAPbI3) and formamidinium lead triiodide (FAPbI3) as absorber perovskite layer in PSCs have been extensively studied [2]. The results have shown that FAPbI3 is thermally more stable which makes it the most promising perovskite material for single-junction PSCs. Recently, rubidium and cesium cations (Rb+ and Cs+) incorporation emerged as a strategy to enhance PSCs efficiency [3]. Following these results, we have synthesised the formamidinium lead triiodide with Rb and Cs ($RbCsFAPbI_3$) as an absorber perovskite layer in PSC device. In this work, we study the factors affecting the $RbCsFAPbI_3$ PSC efficiency by using solar cell capacitance simulator (SCAPS) under AM1.5G illumination.

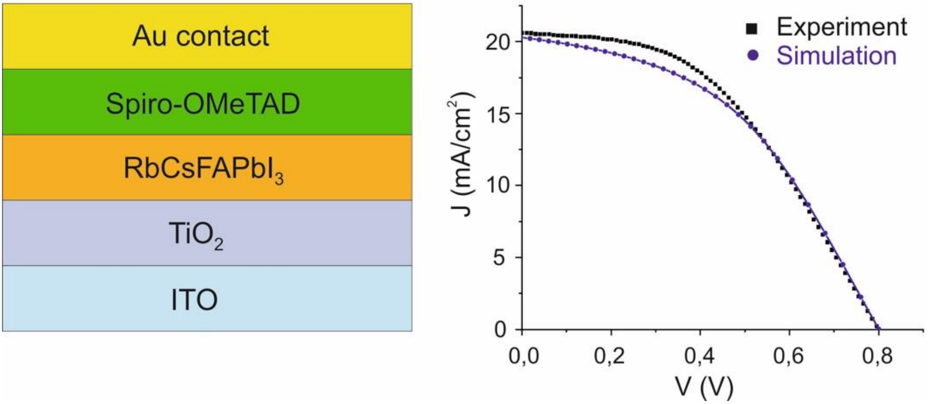

Figure 1. Solar cell structure and I-V characteristics of experimental and simulation data.

[1] A. Kojima et al., *J. Am. Chem. Soc.* **131**, (2009) 6050
[2] N. Pellet et al., *Angew. Chem. Int. Ed*. **53**, (2014) 3151
[3] A. Solanki et al., *Nano Energy* **58**, (2019) 604

This work has been supported by Croatian Science Foundation, IP-2018-01-5246.

P37 - Influence of polyelectrolyte molar mass on formation and properties of PAH/PAA ultra-thin films

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Polyelectrolytes are macromolecules that contain ionic groups in their subunits. Examples of polyelectrolytes are poly(allylamine hydrochloride), PAH, and poly(acrylic acid), PAA. The charge density of these two polyelectrolytes strongly depends on the pH of the solution [1]. In this study, PAH/PAA multilayers on the silicon surface were prepared by the layer-by-layer (LbL) technique [2] using PAH and PAA of two different molar masses (Figure 1). Multilayers were prepared at three different pHs of 5, 8 and 10 with low ionic strength and pH = 8 at high ionic strength. In this way, all 4 conformation combinations that can be obtained with these polyelectrolytes are covered. During the preparation of the multilayer, the thickness of each layer was measured using ellipsometry, and after the multilayer of 10 layers was prepared, its thickness and surface roughness were determined using atomic force microscopy (AFM). The obtained results showed that the molar mass has a greater effect on the thickness of the obtained thin films when the polyelectrolytes are in a globular conformation, while when they are in an elongated conformation, the influence of the molar mass will be smaller.

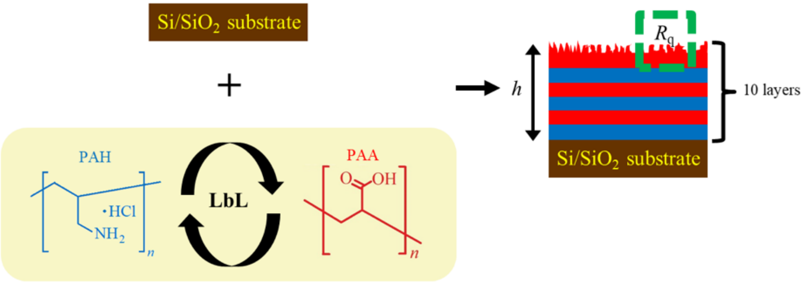

Figure 1 Formation of PAH/PAA multilayer on the Si/SiO_2 substrate.

[1] G. Decher, *Science* **277** (1997) 1232.
[2] J. Choi, M. F. Rubner, *Macromolecules* **38** (2005) 116.

P38 - Homopolymer Of Ladder Flanked with Thiazole: Achieving High-Performance Transport In OTFTs

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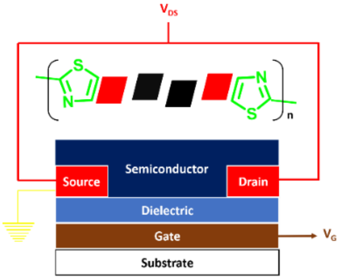
High-performance polymer semiconductors are critical for advancing the field of organic electronics, which relies on the design and synthesis of new electron-deficient (n-type) or electron rich (p-type) building blocks with good solubilizing capability, favorable geometry, and optimized electrical properties. Ladder structures endows a smaller optical bandgap, greater electron delocalization and substantially enhanced electron transport. Consequently, small molecules acceptors have emerged as very important class of compounds consisting typically with ladder structures of fused thiophenes. Homopolymers of ladder monomers with one degree of rotatable bond has been seldom reported, herein we have attempted synthesis of ladder monomer fused with e-deficient thiazole rings flanked at the ends and highly electron rich thienothiophene with pyrrole rings to display a classic donor-acceptor system within a ladder monomer and broadly within the homopolymer. Homopolymers showed p-type semiconducting properties with hole mobility ranging from 0.0068-0.015/$cm^2V^{-1}s^{-1}$.



P39 - NTC Thermistor Properties of Nanocrystalline Fe_2TiO_5

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Iron titanate or pseudobrookite (Fe_2TiO_5), an n-type narrow band gap semiconductor with anisotropic spin glass behavior [1] was synthesized using a modified sol-gel method, with an average grain size of 50 nm [2]. In the temperature range 20-55 °C bulk samples obtained by sintering at 900 °C showed a noticeable NTC thermistor effect, with a $B_{20/55}$ value of 5747 K, and high resistivity of 45 MΩ·cm at 25 °C. A non-linear current-voltage characteristic was obtained at room temperature.

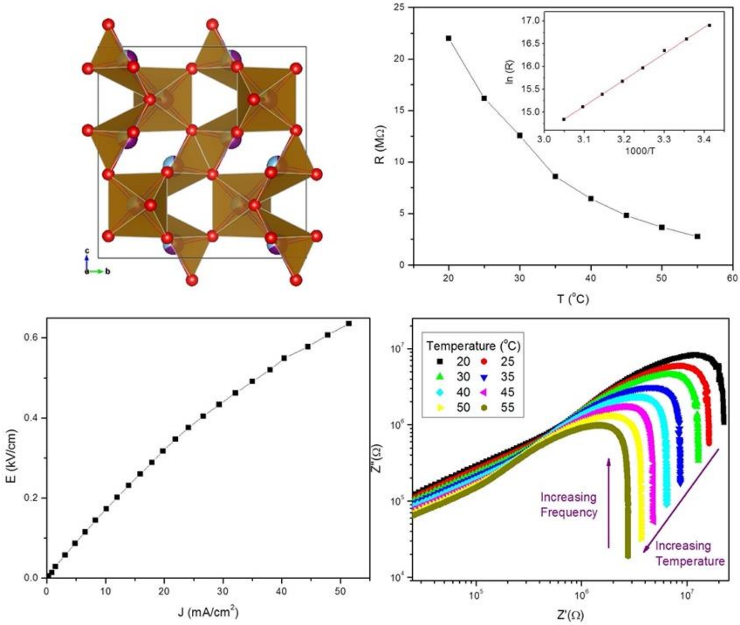

Figure 1 Fe_2TiO_5 crystal structure, DC resistance, complex impedance and I-V response curves.

[1] U. Atzimony, E. Gurewitz, M. Melamud, H. Pinto, H. Shaked, G. Gorodetsky, E. Hermon, R. M. Hornerich, S. Shritkman, B. Wanklyn, *Phys. Rev. Lett.* **43** (1979) 782.

[2] Z. Z. Vasiljevic, M. P. Dojcinovic, J. D. Vujancevic, I. Jankovic-Castvan, M. Ognjanovic, N. B. Tadic, S. Stojadinovic, G. O. Brankovic, M. V. Nikolic, *R. Soc. Open Sci.* **7** (2020) 200708.

P40 - SnSe single crystals: A solid state photodetector and electrochemical photovoltaic study

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Pristine tin selenide (SnSe) possesses desirable optical, thermal, electrical, optoelectronic characteristics for the future nanomaterial of technological applications [1]. In the present study, SnSe single crystals were grown by direct vapour transport (DVT) method. The chemical composition, morphological analysis, crystalline phase, crystallinity, optical properties, vibrational modes and oxidation states of the elements of the grown crystals are verified by EDAX, XPS, optical microscopy-SEM, PL, Raman and X-ray Diffraction. For the optoelectronic study of grown crystals, the current-voltage characteristic was measured. Photodetector based on single-crystalline SnSe is fabricated and studied under visible light with on/off period of 10 sec. The device designates excellent photocurrent and responsivity. Moreover, Photoelectrochemical (PEC) visible light photoresponse of the SnSe single crystals was also studied. The photovoltaic output parameters like the open-circuit voltage (V_{oc}), short circuit current (I_{sc}), fill factor (FF) and efficiency (η%) for the cell were determined. The grown crystal shows the highest photocurrent of 1.31 µA under the illumination of 120 mW/cm^2. Mott-Schottky plots helped in the redox analysis and Energy band location. The Nyquist plot is also plotted to study Electrochemical Impedance. The work demonstrated the potential application of SnSe single crystals in the field of optoelectronic visible light conditions [2].

[1] K. Patel, G. Solanki, K. Patel, V. Pathak P. Chauhan, *Eur. Phys. J. B* **92** (2019) 1.
[2] K. Patel, P. Chauhan, A. B. Patel, G. K. Solanki, K. D. Patel, V. M. Pathak, ACS Appl. Nano Mater. **3** (2020) 11143.

P41 - Fine-tuning of mechanical flexibility of cadmium(II) halide crystals via ligand replacement

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Molecular crystals are excellent candidates for designing a wide range of functional materials due to their arranged internal structure. However, the brittleness and stiffness of the crystals have so far proved to be a limiting factor in their practical implementation. In recent years, there has been an increasing number of molecular crystals that show a flexible response when mechanical force is applied to them, [1,2] but also it has been shown that the degree of mechanical response can be controlled by introducing small structural changes. [3,4] In order to clarify the influence of different structural parameters on mechanical flexibility, we present a new family of coordination cadmium(II) polymers with 2,6-diiodopyrazine, which also show a flexible response to external mechanical force. The molecular and crystal structure were determined and the structural characteristics of the prepared compounds were correlated with the extent of mechanical response.

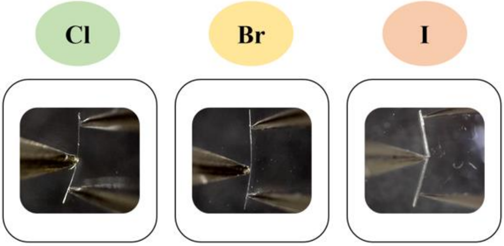

Figure 1. Extent of flexible responsiveness of 1-D cadmium(II) halide polymers with 2,6-diiodopyrazine.

[1] C. M Reddy, G. R Krishna, S. Ghosh, *CrystEngComm* **12** (2010) 2296.
[2] A. Worthy, A. Grosjean, M. C. Pfrunder, Y. Xu, C. Yan, G. Edwards, J. K. Clegg, J. C. McMurtrie, *Nat. Chem.* **10** (2018) 65.
[3] M. Đaković, M. Borovina, M. Pisačić, C.B. Aakeröy, Ž.Soldin, B.-M. Kukovec, I. Kodrin, *Angew. Chem. Int. Ed*. **57** (2018) 14801.
[4] M. Pisačić, I. Biljan, I. Kodrin, N. Popov, Ž. Soldin, M. Đaković, *Chem.Mater.* **33** (2021) 3660.

This work has been fully supported by Croatian Science Foundation under the project IP-2019-04-1242.

P42 - Cu(II) Complexes of 1,2,3-Triazole Linked Dipyridylamine and Ferrocene

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Coordination complexes of dipyridylamine (dpa) have shown interesting properties applicable in catalysis and material sciences as well as medicinal chemistry [1]. Our previous study examined the properties and coordination chemistry of triazole-appended dpa derivatives [2]. To expand the knowledge about this type of ligands, ferrocene derivatives of dpa with 1,2,3-triazole linker and their Cu(II) complexes were prepared. Dpa-tz ligands prefer formation of metal complexes with *trans* configuration, while coordination of the 1,2,3-triazole group depends on N-1 substitution.

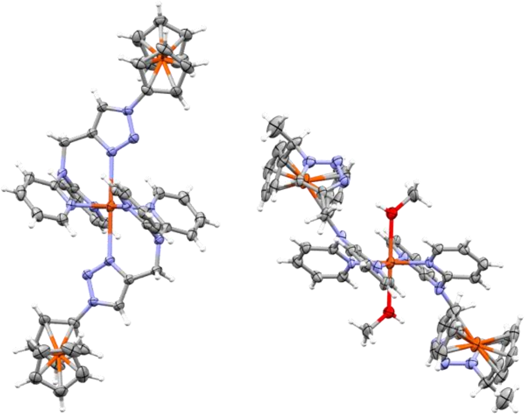

Figure 1. Crystal structures of $[Cu(DpaTzFc)_2](CF_3SO_3)_2$ (left) and $[Cu(DpaTzCHCH_3Fc)_2(MeOH)_2](BF_4)_2$ (right)

[1] S. Wang, C. Bruneau, J. L. Renaud, S. Gaillard, C. Fischmeister, *Dalton Trans.* **48** (2019) 11599.
[2] N. Pantalon Juraj, M. Krklec, T. Novosel, B. Perić, R. Vianello, S. Raić-Malić, S. I. Kirin, *Dalton Trans.* **49** (2020) 9002

P43 - Coordination polymers of the {MoO_2^{2+}}-dihydrazone type as structurally and topologically versatile systems

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Dioxomolybdenum(VI) complexes based on dihydrazone scaffolds have proved well their coordination and supramolecular prospects for the design of materials ranging from discrete multinuclear complexes to polyoxometalates.[1] In contrast to their rigid benzhydrazones and carbohydrazone congeners, alkyl (di)hydrazones offer entirely new scenarios when considering materials framework topology. As we show, the extreme topological richness can be achieved by combining flexible alkyl (di)hydrazones with rigid bis(pyridyl) linkers, while relying on the coordinatively predictable MoO_2^{2+} core. A detailed structural analysis unveils that the geometrical features and topology of the polymers are dictated by the conformational flexibility of the alkyl chain of the ligand, as well as hydrogen-bonding propensities of peripheral functional groups.

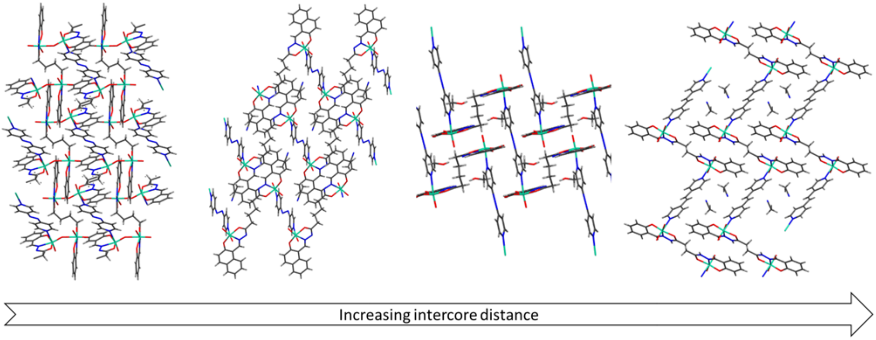

Figure 1. Crystal packing in four selected coordination polymers. The geometry of packing is dictated by the conformation of the ligand and the presence of peripheral functional groups.

[1] E. Topić, I. Landripet, M. Duguin, J. Pisk, I, Đilović, V. Vrdoljak, M. Rubčić, *New J. Chem* **44** (2020) 13357; E. Topić, J. Pisk, D. Agustin, M. Jendrlin, D. Cvijanović, V. Vrdoljak, M. Rubčić, *New J. Chem* **44** (2020) 8085.

P44 - Sustainability of the robust pyridone homosyntone in halogen-bonded cocrystals

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It is well known that species containing 2-pyridone (pdon) fragment easily undergo tautomerization process which includes two tautomeric forms – lactame and lactime [1]. In solid state, both tautomers can aggregate in robust hydrogen-bonded dimers by pyridone homosynthon involving two N–H···O or O–H···N hydrogen bonds [2]. Constancy of such dimers is well described in papers dealing with multicomponent hydrogen-bonded systems [3], while their coexistence with halogen bonds in organic solids has not been noticed to date. To investigate hierarchy of supramolecular interactions in such systems, we synthesized a series of halogen-bonded cocrystals of 2-pyridone and perhalogenated hydrocarbons. In all 6 prepared compounds, 2-pyridone is present in lactame form and expectedly connected in centrosymmetric dimers through two N–H···O hydrogen bonds. Corresponding perhalogenated donors participate in I···O halogen bonding, thus forming discrete molecular complexes (1 case) or supramolecular chains (5 cases).

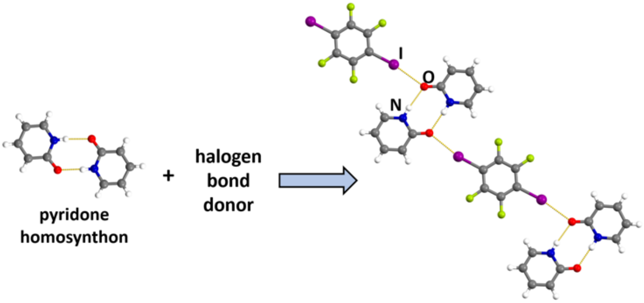

Figure 1. Halogen and hydrogen bonding in (pdon)(14tfib).

[1] H. W. Yang, B. M. Craven *Acta. Cryst.* B**54** (1998) 912.
[2] J. Almlöf, A. Kvick, I. Olovsson *Acta. Cryst.* B**27** (1971) 1201.
[3] C. B. Aakeröy, A. M. Beatty, M. Zou *Cryst. Eng.* **1** (1998) 225.

P45 - Halogen bonding in salts of ortho-halogenpyridines and hexacyanocobaltate(III) acid

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Cyanometallate anions such as hexacyanoferrate or hexacyanocobaltate are Lewis bases and are therefore good hydrogen [1] and halogen bond [2] acceptors. Protonated cyanometallate anions, such as hexacyanoferrates, are good hydrogen bond donors.[3] Protonated hexacyanoferrates have recently also been studied as potential halogen bond donors.[4] To the best of our knowledge, no similar studies have been performed with other protonated cyanometallates to date.

In this work we have used hexacyanocobaltate(III) acid ($H_3[Co(CN)_6]$) with 2-chloropyridine (2-Clpy), 2-bromopyridine (2-Brpy) and 2-iodopyridine (2-Ipy) to synthetize three salts. In all three cases I···N halogen bonds and N-H···N hydrogen bonds are present, along with O-H···N hydrogen bonds between the anions and Zundel ($H_5O_2^+$) cations. The anion is completely deprotonated in all three salts. 2-Clpy and 2-Brpy salts are isostructural, while the 2-Ipy salt contains a tetramer of water molecules bridging six hexacyanocobaltate(III) anions and two 2-IpyH cations.

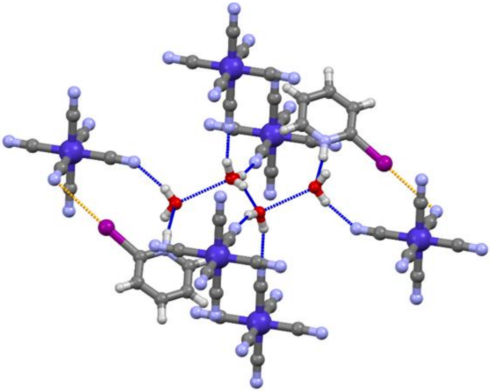

Figure 1 Tetramer of water molecules in $(H_5O_2)(2\text{-IpyH})_2[Co(CN)_6](H_2O)_2$.

[1] B. Yan, H. D. Wang, Z. D. Chen, *J. Mol. Struct.*, **569** (2001) 65.
[2] J. E. Ormond-Prout, P. Smart, L. Brammer, *Cryst. Growth. Des.*, **12** (2012) 205.
[3] I. Cvrtila, V. Stilinović, *Cryst. Growth Des.*, **17** (2017) 6793.
[4] N. Jakupec, L. Fotović, V. Stilinović, *CrystEngComm*, **22** (2020) 8142.

P46 - ***Salen* complexes as halogen bond acceptors**

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Imine complexes are good halogen bond acceptors towards classical halogen bond donors (i.e. perfluorinated iodobenzenes) [1]. *Salen* complexes, a special class of compounds within imine complexes, were found to generally act as hydrogen bond or cation receptors [2], while they have not been explored to an equal extent as potential halogen bond acceptors [3].

In order to investigate the preference of metal *salen* complexes as halogen bond acceptors towards perfluorinated iodobenzenes, we have cocrystallized nickel *salen* complex (NiL) with 14tfib in the solid state and in solution. The solid state reaction was preformed mechanochemically either with NiL and the 14tfib, or with the mixture of *o*-phenylenediemine, *o*-vanillin, nickel(II) acetate and 14tfib, so that the formation of the ligand, its complexation of nickel and formation of the cocrystal occurs in a single-pot mechanochemical reaction. In both cases the same product was obtained. Single crystals of the same product were obtained from the solution synthesis, and have shown to be a $(NiL)_2(14tfib)$ cocrystal, in which iodine acts as a halogen bond donor towards three oxygen atoms in the complex.

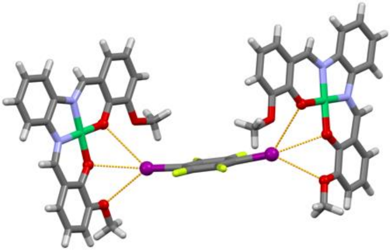

Figure 1 Discrete motif in $(NiL)_2(14tfib)$ cocrystal.

[1] V. Nemec, K. Lisac, N. Bedeković, L. Fotović, V. Stilinović, D. Cinčić, *CrystEngComm* **23** (2021) 3063.
[2] M. Andruh, D. G. Branzea, R. Gheorghe, A. M. Madalan, *CrystEngComm* **11** (2007) 2571.
[3] Q. Wu, J.-C. Xiao, C. Zhou, J.-R- Sun, M.-F. Huang, X. Xu, T. Li, H. Tian, *Crystals* **10** (2020) 334.

P47 - Cocrystals of nickel(II) coordination compounds with perhalogenated halogen bond donors

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In the last decade, neutral metal-organic compounds containing halogenide ligands as halogen bond acceptors have proven to be reliable building blocks in the design and syntheses of halogen-bonded metal-organic cocrystals [1]. Following our previous studies, where the halogen bonding proclivity of the chlorine atom coordinated to the Co(II) metal centre in metal-organic halogen bonded cocrystals was described [2,3], in this work we have explored the ability of $NiCl_2L_2$ metal complexes (L = 2-acetylpyridine, 2-benzoylpyridine) to act as halogen bond acceptors with six perhalogenated organic compounds as halogen bond donors. By grinding combinations of the two Ni(II) complexes with the selected donors, we obtained nineteen new phases, and five cocrystal single crystals were obtained by crystallization from solution. X-ray structural analysis revealed that the dominant supramolecular interaction in all cocrystals is the Ni–Cl···I halogen bond between halogen bond donor iodine atoms and Ni(II) complex chlorine atoms.

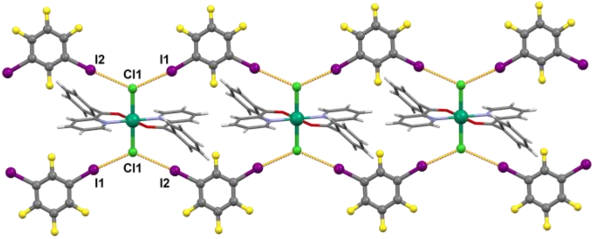

Figure 1 Halogen bonded chain in the cocrystal of *trans*-bis(2-benzoylpyridine)dichloridonickel(II) with 1,3-diiodotetrafluorobenzene

[1] V. Nemec, K. Lisac, N. Bedeković, L. Fotović, V. Stilinović, D. Cinčić, *CrystEngComm* **23** (2021) 3063.
[2] K. Lisac, D. Cinčić, *CrystEngComm* **20** (2018) 5955.
[3] K. Lisac, D. Cinčić, *Crystals* **7** (2017) 363.

P48 - Improving solid-state and biopharmaceutical performance of haloperidol via salt formation with dicarboxylic acids

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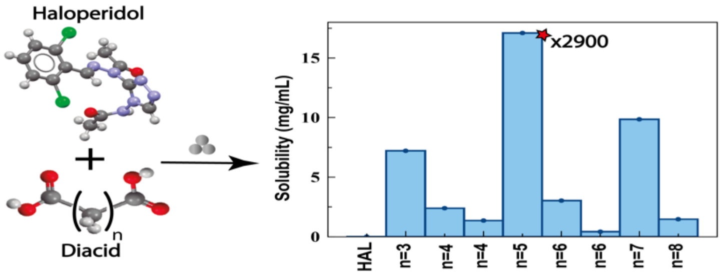
Crystal engineering has provided an efficient approach for tuning physicochemical properties of active pharmaceutical ingredients (APIs), and therefore has a direct application in the pharmaceutical industry. For instance, salt formation is a widely used strategy to improve the solubility of ionizable drugs [1].

In this work we have conducted a systematic study to evaluate the impact of counterions on the solid-state performance of pharmaceutical salts of haloperidol. Crystalline salts were synthesized using haloperidol and a series of closely related (di)carboxylic acid counterions. Eight new pharmaceutical salts were prepared by mechanochemical methods and characterized by thermal, spectroscopic and diffractometric techniques. Their crystal structures have been determined to evaluate the role of intermolecular interactions on the improvement of physicochemical properties. Stability studies at 40 ºC and 75% RH as well as their solubility determination contributed to complete the whole picture of these multicomponent molecular materials.



[1] Kasim, N. A.; Whitehouse, M.; Ramachandran, C.; Bermejo, M.; Lennerna, H.; Hussain, A. S.; Junginger, H. E.; Stavchansky, S. A.; Midha, K. K.; Shah, V. P.; Amidon, G. L. Mol. Pharmaceutics, **1** (2004) 85.

P49 - Schiff bases as halogen bond donors in crystal engineering of cocrystals

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In the past two decades, halogen bonding has been shown as an effective and predictable tool in crystal engineering [1]. It has been predominantly investigated in multicomponent crystals consisting of organic perhalogenated compounds as halogen bond donors and various organic and metal-organic compounds as halogen bond acceptors [2]. While many multicomponent systems contain Schiff bases as halogen bond acceptors [3], there are scarce examples of those that contain them as halogen bond donors [4]. In this work, we have prepared two peripherally perhalogenated Schiff bases by reaction of 2,3,5,6-tetrafluoro-4-iodoaniline with salicylaldehyde (itfasal) or *ortho*-vanillin (itfaovan). Both Schiff bases were cocrystallized in 2:1 molar ratio with selected acceptors: 4,4’-bipyridine (bpy), 1,4-diazabicyclo[2.2.2]octane (dabco) and 1,2-bis(4-pyridyl)ethane (bpean). Cocrystals were prepared by liquid-assisted grinding and crystallization from ethanol and characterized by X-ray diffraction methods. Structural characterization revealed that in all six cocrystals itfasal and itfaovan are bonded with acceptors *via* I···N halogen bonds.

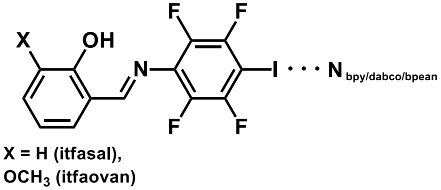

Figure 1 Halogen-bonded Schiff base with an acceptor nitrogen atom.

[1] G. Cavallo, P. Metrangolo, R. Milani, T. Pilati, A. Priimagi, G. Resnati, G. Terraneo, *Chem. Rev.* **116** (2016) 2478.
[2] C. R. Groom, I. J. Bruno, M. P. Lightfoot, S. C. Ward, *Acta Cryst. B* **72** (2016), 171.
[3] A. Carletta, M. Zbačnik, M. Vitković, N. Tumanov, V. Stilinović, J. Wouters, D. Cinčić, *CrystEngComm* **36** (2018), 5332.
[4] Y. Wang, H. Shang, B. Li, H. Zhang, S. Jiang, *CrystEngComm* **19** (2017) 3801.

P50 - Investigation of Physicochemical Property of Favipiravir Cocrystal with Theophylline and GRAS Coformers

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Five cocrystals of antiviral drug favipiravir (Fav) with respiratory drug theophylline (Theo) and GRAS coformers viz. p-aminobenzoic acid (PABA), 4-hydroxybenzoic acid (4HBA), gallic acid (GA) and ferulic acid (FRA) were successfully synthesized using mechanochemistry as well as solution crystallization (Figure 1).[1] All the synthesized cocrystals were characterized using PXRD, SCXRD and thermal measurements. Equilibrium solubility study showed that the trend in cocrystal solubility nicely correlates with coformer solubility. Also the solubility can be tuned based on coformer selection during co-crystallization process. Crystal structure analysis depicts amide-amide homosynthon formation in Fav•Theo cocrystal, whereas acid-amide heterosynthon in case of cocrystals with GRAS coformers. The drug-drug cocrystal Fav•Theo might be a potential formulation for patients suffering from viral infection such as COVID-19 along with asthma or chronic obstructive pulmonary disease (COPD) related respiratory syndrome.

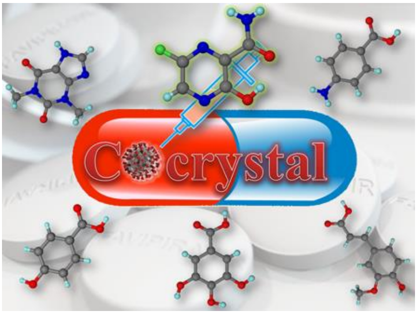

Figure 1. Favipiravir cocrystal considered for our study.

[1] P. Deka, D. Gogoi, D. R. Rao, R. Thakuria, *Cryst. Growth Des,* (2021) Under Revision.

P51 - 2D arrays of pancake-bonded oligomers of TCNQ radicals

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Multicentric two-electron (mc/2e) bonding between 7,7,8,8-tetracyanoquinodimethane (TCNQ) radical anions was studied on its 14 salts with planar organic cations. Formal charges of the TCNQ moieties are -1/2 and -2/3, and they form mc/2e bonded dimers, trimers and tetramers which are further stacked in extended arrays (Fig. 1). Multicentric bonding (*pancake bonding*) within these oligomers is characterised by short interplanar separations of 2.9 - 3.2 Å; distances between the oligomers are larger, typically > 3.3 Å. The stacks are laterally connected by C–H···N hydrogen bonding, forming 2D arrays. Nature of mc/2e bonding is studied by structural, magnetic and electrical characterisation. The compounds are found to be semiconductors, and high conductivity (10^{-2} Scm^{-1}) was correlated with shorter interplanar distances between pancake-bonded oligomers.

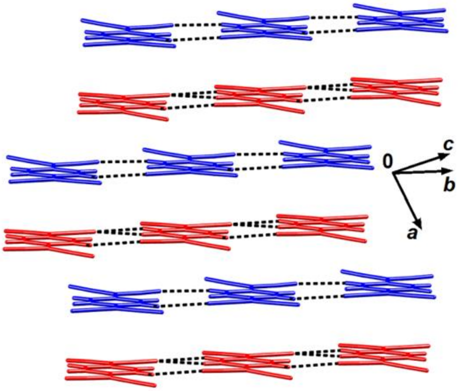

Figure 1 2D array of pancake-bonded dimers of TCNQ radical anions in its salt with 4-iodo-*N*-methylpyridinium. Two symmetry-independent TCNQ moieties are shown as red and blue.

P52 - Self-assembly of diamondoid ethers on graphite

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Diamondoids are natural polycyclic cage hydrocarbons with a structure resembling the diamond crystal lattice [1]. Despite being structurally similar to diamond, diamondoids have a marked advantage over it since they can be selectively functionalized, making them applicable in areas ranging from medicine [2] to nanotechnology [3]. As part of our ongoing research, we synthesized diamondoid ether derivatives differing in the type, size and number of their cage subunits. Conducted STM/AFM measurements demonstrated the organization of diamondoid ether molecules on a graphite substrate (HOPG) and revealed the existence of self-assembled 2D layers. Comparing these 2D assemblies with crystal structures obtained from single-crystal XRD experiments and with computed models, we could ascertain London dispersion as a driving force for self-organization of such bulky molecules on a HOPG carrier surface.

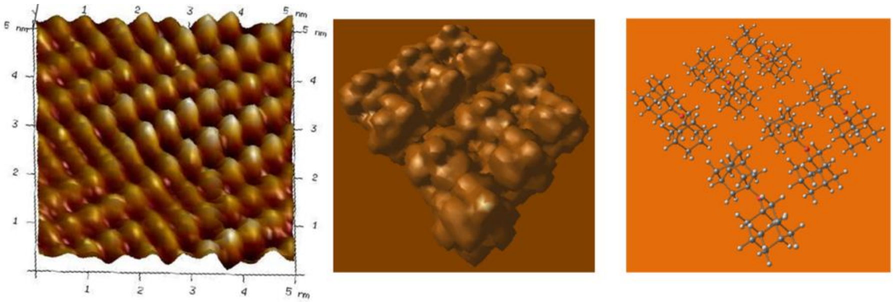

Figure 1 STM image of di(1-adamantyl) ether on a HOPG (left) compared with DFT computed electron density (middle) obtained from ether structures (right).

[1] A. A. Fokin, P. R. Schreiner, H. Schwertfeger, *Angew. Chem. Int. Ed.* **47** (2008) 1022.
[2] L. Wanka, K. Iqbal, P. R. Schreiner, *Chem. Rev.* **113** (2013) 3516.
[3] H. Y. Gao, M. Šekutor, L. Liu, A. Timmer, H. Schreyer, H. Mönig, S. Amirjalayer, N. A. Fokina, A. Studer, P. R. Schreiner, H. Fuchs, *J. Am. Chem. Soc.* **141** (2019) 315.

P53 - Design and characterization of azo-linked porous organic polymers

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Porous organic polymers (POPs) are solid materials which are built by covalently linking organic molecular building blocks of different geometries and topologies [1]. Characteristics of POPs such as large specific surface area, high porosity, high chemical and thermal stability and low density, make them suitable for a range of applications, especially in gas storage and separation. For example, POPs containing azo linkages were found to exhibit high affinity for CO_2 uptake and low affinity towards N_2, making them as good candidates in post-combustion CO_2 capture and for highly selective gas separations [2].

In the present study, we synthesized several new azo-linked polymers by coupling of 1,3,5-tris(4-nitrophenyl)benzene with various aromatic diamino compounds, differing in length and rigidity, under basic conditions. The obtained polymers are insoluble in common organic solvents. IR and ^{13}C CP/MAS NMR spectroscopy suggested formation of azo linkages and the presence of nitro and amino end-groups. Powder XRD data revealed amorphous nature of azo polymers while TG analysis indicated their very high thermal stability. DFT study revealed the most probable sites of interaction between the building units connected by azo bonds and gas molecules of CO_2 and N_2. Binding energies were calculated for both aromatic and azo groups to delineate their effects on CO_2/N_2 selectivity of the synthesized POPs.

[1] S. Das, P. Heasman, T. Ben, S. Qiu, *Chem. Rev.* **117** (2017) 1515.
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P54 - Al sites in CHA-type zeolite materials

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CHA-type zeolites are commercial catalysts in the exhaust gas treatment for the SCR of NO_x and in the MTO technology [1, 2]. Still, there is a demand to develop more environment-friendly synthesis routes and improve their performance in these processes as well as in other potential applications. Acidic properties and the distribution of Al species represent crucial features that define the efficiency of zeolite catalysts. Herein is studied the correlation between the synthesis conditions of a series of SSZ-13 zeolite materials and their respective properties. The materials were prepared using commercial FAU-type zeolite, NaOH or KOH, TMADAOH and water. The features of the prepared materials were evaluated by powder X-ray diffraction, scanning electron microscopy, dynamic light scattering, thermogravimetric analysis, UV–VIS spectroscopy, nitrogen adsorption/desorption, as well as nuclear magnetic resonance, atomic absorption and infrared spectroscopy.

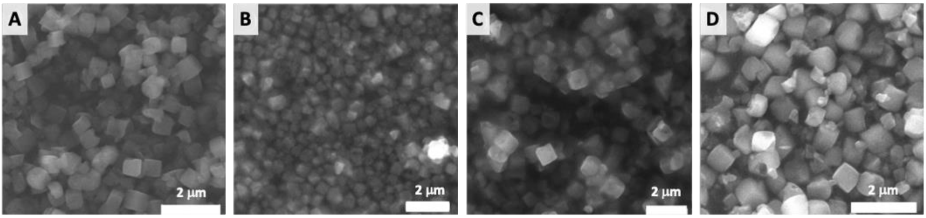

Figure 1 Scanning electron microscope micrographs of a studied series of CHA-type zeolite materials prepared in KOH medium.

[1] R. Zhang, N. Liu, Z. Lei, B. Chen, *Chem. Rev.* **116** (2016) 3658.
[2] M. Dusselier, M. E. Davis, *Chem. Rev.* **118** (2018) 5265.

P55 - Integration of Glycosaminoglycans within Metal-azolate frameworks

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[1]A Graz University of Technology, Institute of Physical and Theoretical Chemistry,
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The integration of biomacromolecules within a MOF-shell can be achieved by inducing the spontaneous formation of the MOF matrix around the target biomolecule [1]. The most studied matrices for the synthesis of biomacromolecules@MOFs are metal-azolate frameworks (MAFs). The widespread interest in MAF-based biocomposites is justified by their high encapsulation efficiency, high thermal stability, and their triggered-drug release properties. In this work, [2] we encapsulated different glycosaminoglycan-based therapeutics (GAG = heparin, hyaluronic acid, chondroitin sulfate, dermatan sulfate) in three different MAFs such as ZIF-8, ZIF-90, and MAF-7. The resultant GAG@MAF biocomposites exhibit significant differences in terms of crystallinity, particle size, and spatial distribution of the cargo. These features have a direct influence on the drug-release kinetics upon applying an acidic stimulus, as well as in the bio- protection capabilities of the MOF-shell. Overall, the present work demonstrates that by varying the identity of the MOF-shell we can tune the release profile, the encapsulation efficiency, and the biopreservation of the target biomacromolecule.

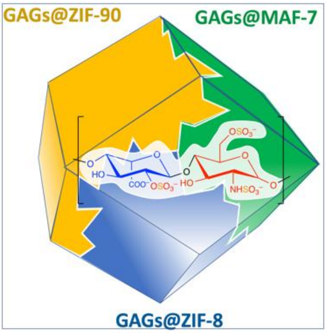

Figure 1. ***GAGs@MAFs***

[1] M. de J. Velásquez-Hernández, M. Linares-Moreau, E. Astria, F. Carraro, M. Z. Alyami, N. M. Khashab, C. J. Sumby, C. J. Doonan, P. Falcaro, *Coord. Chem. Rev.*, **429** (2021) 213651.
[2] M. de J. Velásquez-Hernández, E. Astria, S. Winkler, W. Liang, H. Wiltsche, A. Poddar, R. Shukla, G. Prestwich, J. Paderi, P. Salcedo-Abraira, H. Amenitsch, P. Horcajada, C. J. Doonan, P. Falcaro, *Chem. Sci.*, **11** (2020) 10835.

P56 - Bimetallic MOF-74 Catalysts for Selective Hydrogenation of CO_2 to Methanol

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Carbon capture and storage technologies can significantly reduce our need for fossil fuels. Hydrogenation of CO_2 to methanol over a mixed-metal $Cu/ZnO/Al_2O_3$ catalyst is a promising industrial process that can efficiently use CO_2.[1] However, to further increase the selectivity of the process, new catalytic materials are being investigated.

We wanted to determine whether the high porosity and accessibility of metal nodes in ZnCu-MOF-74 make this MOF suitable for this purpose. The catalysts were prepared by ball milling, which allows stoichiometrically controlled preparation of bimetallic ZnCu-MOF-74 materials.[2] The catalytic performance of the prepared ZnCu-MOF-74, monometallic Cu-MOF-74, and industrial $Cu/ZnO/Al_2O_3$ catalyst were evaluated. In addition, to assess whether the collapse of the porous structure of MOF-74 via mechanochemical amorphization may contribute to catalytic activity and selectivity, amorphized ZnCu-MOF-74 was also examined. Bimetallic MOF-74 was found to have better catalytic properties than monometallic one, while mechanochemical amorphization strongly affects both the catalytic activity and the selectivity of the bimetallic MOF-74 catalyst.[3]

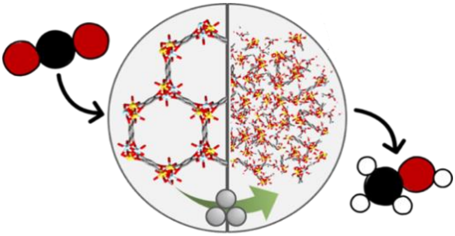

Figure 1. Crystalline and mechanochemically amorphized ZnCu-MOF74 material for catalytic hydrogenation of CO_2 to methanol

[1] A. Goeppert et al. *Chem. Soc. Rev.***43** (2014) 7995
[2] G. Ayoub et al. *Chem. Mater*. **31** (2019) 5494.
[3] T. Stolar et al., *ACS Appl. Mater. Interfaces* **13** (2021) 3070.

P57 - Controllable Encapsulation of Fullerene-C_{60} into the small-aperture pore of ZIF-8 by Ball Milling

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Metal-organic frameworks (MOFs) are an important class of porous materials for many application areas. Merging the unique structural properties of MOFs with intrinsic properties of fullerenes, such as electron-accepting properties and fast electron transfer, gives the opportunity to investigate new class fulleretic materials for their potential application areas such as the development of molecular electronics, photosensitizer, catalysis, etc. However, the majority of the encapsulation processes are based on post-synthetic methods, such as soaking, which results in an uncontrollable and low amount of loading due to the size of the apertures and solubility. Here we present a rapid, green, efficient, and controllable solvent-free ball-milling method to encapsulate and immobilize fullerene C_{60} guests into the sodalite phase of zeolitic imidazole framework-8 (ZIF-8) MOF to obtain fulleretic materials with a controllable amount of guests in the pores. [1] Computational and spectroscopic studies clarify that the movement of fullerene between the pores is energetically unfavoured.

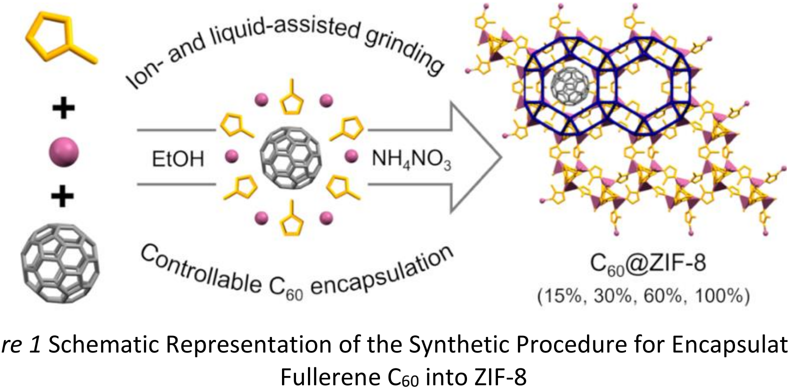

Figure 1 Schematic Representation of the Synthetic Procedure for Encapsulation of Fullerene C_{60} into ZIF-8

[1] V. Martinez, B. Karadeniz, N. Biliškov, I. Lončarić, S. Muratović, D. Žilić, S. M. Avdoshenko, M. Roslova, A. A. Popov, K. Užarević, *Chem. Mater*. **32** (2020), 10628.

P58 - Influence of π-Spacer Heterocycle in the Homopolymer Optoelectronic Properties

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Polymeric conjugated materials, or conductive polymers, are organic polymers having conductivities similar to metals or semiconductors due to their continuous π-conjugated double bonds. However, unlike metals or inorganic semiconductors, this type of materials is essentially like plastics, having the advantage of processability. Moreover, their properties could be finely tuned with related monomers structure designs. As a successful strategy in polymer photovoltaic materials, pull–push mode of structures, containing electron-pulling and pushing units, have been widely adapted to provide more efficient intramolecular charge transfer (ICT) and adjustments of the bandgaps and energy levels of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO).[1]

The effect of lateral heterocycles on the final monomer can play an important role in the polymerization reaction, as well as can affect optical, electrochemical and morphological properties of the homopolymer as a thin film.[2]

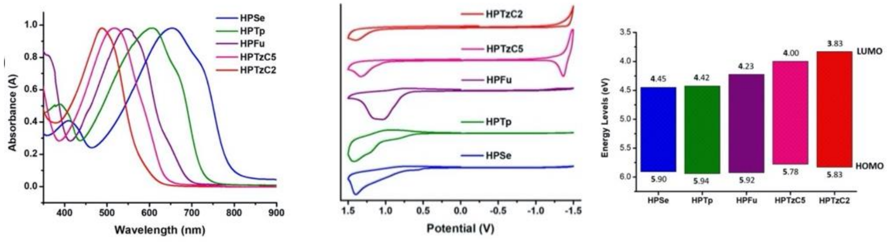

Figure 1 UV-vis absorption spectra, cyclic voltammograms and energy levels of the homopolymers.

[1] M. Comí, D. Patra, R. Yang, Z. Chen, A. Harbuzaru, Y. Wubulikasimu, S. Banerjee, R. Ponce Ortiz, Y. Liu M. Al-Hashimi. *J. Mat Chem. C.* **9** (2021) 5113.

[2] M. Comí, M. U. Ocheje, S. Attar, A. U. Mu, B. K. Philips, A. J. Kalin, K. E. Kakosimos, L. Fang, S. Rondeau-Gagné M. Al-Hashimi. *Macromolecules* **54** (2021) 665.

P59- Ionic cocrystals derived from 3-halogenpyridinium halogenides and perfluorinated iodobenzenes

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The halogen bond presents a highly directional class of intermolecular interaction frequently employed in crystal engineering [1]. The usage of neutral halogen bond acceptors in supramolecular systems is very well established, while anionic acceptor species are considerably less represented. Halogenide ions have been proven to be good halogen and hydrogen bond acceptors, because of the large charge concentration on one atom [2]. In this work, halogenpyridinium salts, 3-chloro- and 3-bromopyridinium chloride and bromide have been successfully cocrystallized with two geometrically different perfluorinated halogen bond donors: 1,4-diiodotetrafluorobenzene (**14tfib**) and 1,2-diiodotetrafluorobenzene (**12tfib**). Using halogenide ions as templates for the formation of halogen and hydrogen bonded multi-component systems, series of 8 cocrystals was obtained in which 3 pairs of isostructural cocrystals were formed.

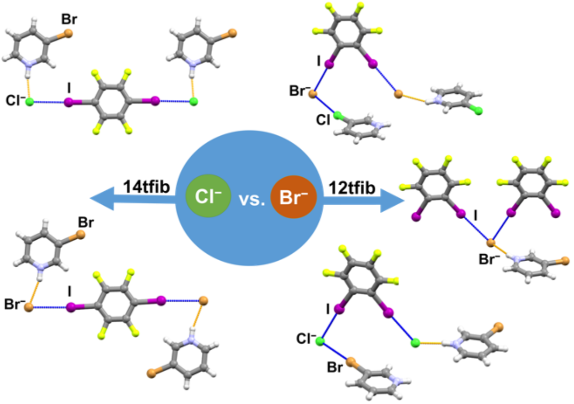

Figure 1. Discrete halogen and hydrogen bonded units prepared in this work

[1] G. Cavallo, P. Metrangolo, R. Milani, T. Pilati, A. Priimagi, G. Resnati, G. Terraneo, *Chem. Rev.*, **116** (2016) 2478.
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P60 - Synthesis and structural characterization of the oxalate-based compounds with alkyl ammonium cations

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Multifunctional properties of the metal-organic coordination polymers can be achieved by combining the intrinsic properties of the host, especially the magnetic ones, with an additional functionalities coming from the selected guest molecules. The oxalate group, $C_2O_4^{2-}$, has been demonstrated to be one of the most versatile ligands used in the preparation of these systems. Due to its various coordination modes towards the metal centres as well as its ability to mediate magnetic interactions between paramagnetic metal ions, a large number of oxalate-based transition-metal species of different nuclearity, connectivity and dimensionality have been synthesized and characterized, many of them having tunable magnetic frameworks. Furthermore, the simplest method to obtain conductive compound is to introduce proton carries directly as counterions such as NH_4^+, H_3O^+ and to make proton-conducting pathways composed of hydrogen-bond networks [1].

In previous work, we reported one-dimensional antiferromagnetic oxalate-bridged coordination polymer $\{[NH(CH_3)_2(C_2H_5)][FeCl_2(C_2O_4)]\}_n$, showing hydrogen-bonded diethylmethylammonium cationic moieties what lead to a very high room-temperature proton conductivity [2.70×10^{-4} $(\Omega\ cm)^{-1}$ under 93% relative humidity conditions]. Therefore, we have continued to prepare oxalate systems containing various alkyl ammonium cationic components, with the aim of obtaining compounds which, in addition to interesting magnetic properties, also show proton conductivity. In order to obtained such heterometallic complexes, tris(oxalato)metalates, $[M^{III}(C_2O_4)_3]^{3-}$ (M^{III} = Cr or Fe), are used as ligands towards second transition metal ion.

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P61 - Stacking patterns of TCNQ radical anions in different salts with organic cations

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π-stacking is a well-known type of intermolecular interaction which occurs usually between aromatic rings, but also between non-aromatic π-systems. It is considered mostly as weak interaction; however recent studies show that energy of such contacts may be as high as energy of strong intermolecular interactions. Therefore, π-stacking has an important role in crystal engineering of functional materials such as optoelectronics, magnetic and conductive molecular materials. [1] Herein we have studied stacking of 7,7,8,8-tetracyanoquinodimethane (TCNQ) radical anions on its 6 diverse salts with organic cations: tetrazolium, 2-amino-5mentil-N-methylpyridinium, N-ethyl-2-methylpyridinium, 1,4-dimethyl-DABCO cation, 2-chloro-N-methylpyridinium and 2-aminopyridinium cations. Formal charges of TCNQ moieties in these salts are -1/2, -2/3 and -4/5. They form stacks with alternating shorter and longer separation between TCNQ rings (dimers or trimers) or stacks in columns with equidistant separations (Fig 1). In these compounds stacking interactions are predominant with interplanar separations between rings of 3,0 – 3,3 Å. Furthermore, in some salts between components N–H···N and C–H···N hydrogen bonds are present.

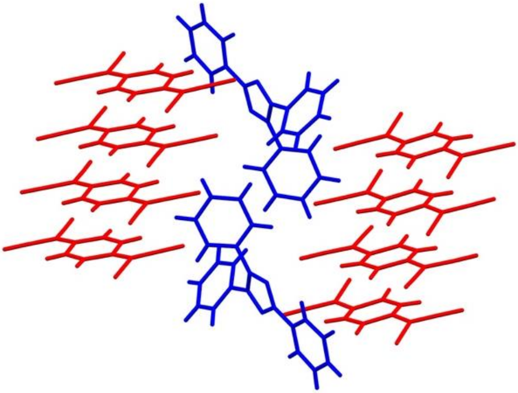

Figure 1 Stacking of TCNQ radical anions in salt with tetrazolium cation.

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P62 - ROMP of thioether functional oxanorbornene imide and its copolymerization with various cyclic comonomers

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Ring opening metathesis polymerization (ROMP) is a remarkable alternative method for preparing functional polyolefins.[1-3] Here, we present the synthesis of novel thioether-functional poly(olefin)s *via* the ROMP of thioether-functionalized oxanorbornene imide (**M1**) and its copolymerization with cyclic comonomers such as cyclopentene (**M2**), cyclopent-3-en-1-ol (**M3**), cycloheptene (**M4**) and cyclooctene (**M5**) using Hoveyda-Grubbs 2nd generation Ru-catalyst **HG2**. The time-depended ^{1}H NMR experiments displayed the reactivity and the influence of temperature on the conversion of each monomer in the metathesis polymerization. A five membered cycloolefin monomer **M2** showed low ROMP reactivity at 0 °C or 25 °C in the copolymerization. Apparently, the percentage of monomer incorporation in the isolated poly(olefin)s were determined in the order of **M5>M3>M4>M1**. Isolated polymer yields were ranging from 69-70% and 38-92% respectively for the polymerizations carried out at 0 °C and 25 °C. Additionally investigated the molecular weights (M_n) and thermal properties of poly(olefin)s.[4]

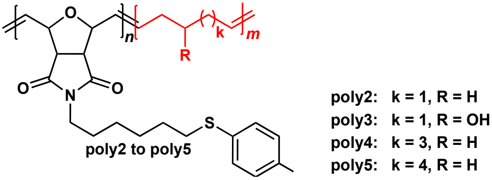

Figure 1 Poly(oxanorbornene imide) based copolymers.

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P63 - Synthesis and characterization of a novel chiral coordination polymer of copper(II) with L-proline

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Chiral coordination polymers (CPs) are a group of compounds of great interest due to their potential applications in various areas where enantioselective binding is required [1]. A novel chiral CP of copper(II) and 4,4'-bipyrdine with L-proline, was synthesized and structurally characterized using single crystal diffraction (SCXRD). Large channels, 11 Å in diameter, are present in the crystal structure of the prepared compound. The compound was studied using thermogravimetric analysis coupled with infrared spectroscopy (TGA/DSC-FTIR) and temperature dependent powder X-ray diffraction (TPXRD). It was determined that the CP framework is robust up to 110 °C (Figure 1). In the range of 110 – 150 °C, minute amounts of decomposition products are formed. At higher temperatures, the compound fully decomposes yielding copper(II) oxide. TGA/DSC-FTIR analysis shows that the solvent present in the channels is continuously released as the temperature increases. The CP has a rare chiral **uon** topology [2, 3].

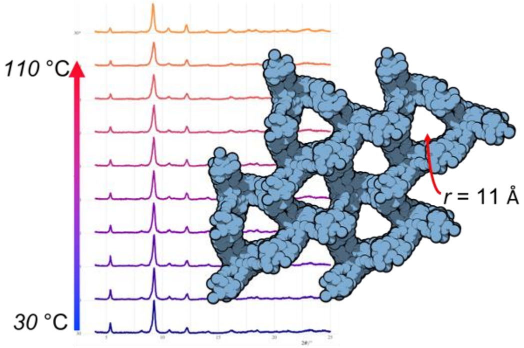

Figure 1 Crystal packing along the crystallographic c axis showing only the CP framework (blue) and the TPXRD diffractograms.

[1] J. S. Seo, D. Whang, H. Lee, S. I. Jun, J. Oh, Y. J. Jeon, K. Kim, *Nature* **404** (2000) 982.
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[3] V. A. Blatov, A. P. Shevchenko, D. M. Proserpio, *Cryst. Growth Des.* **14** (2014) 3576.

P64 - Theoretical and experimental characterization of ferrocene tripeptides

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Organic chromophores can be used as the sensing elements for determination of the helicity of small peptides.[1,2] The screw sense of the helix is correlated with the sign of the Cotton effect in circular dichroism (CD) spectra. Our group's studies have shown that even small monosubstituted peptidomimetics derived from ferrocenamine show a signal in the CD spectra near 470 nm related to the ferrocene chromophore region.[3]

Two novel stereoisomeric ferrocene-based tripeptides, Boc-Pro-Pro-Ala-NHFc, were synthesized and characterized experimentally (IR, NMR, CD). Theoretical conformational analysis performed in implicitly modelled solvent, nicely corroborates with the experimental findings about the hydrogen bond patterns. Varying in the chirality of only one amino acid, two stereoisomers show a significantly different distribution of the conformers. In both stereoisomers dominates only *P*-helix, although the unique orientation of the ferrocene subunit pointing away from the peptide chain is obtained in stereoisomer with heterochiral Pro-Pro amino acid sequence. A strong correlation was also noticed between the sign of the Cotton effect and dihedral angle describing the deviation between the amide and cyclopentadienyl ring plane.

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P65 - Biodegradation of PS and PVC microplastics by Bacillus cereus

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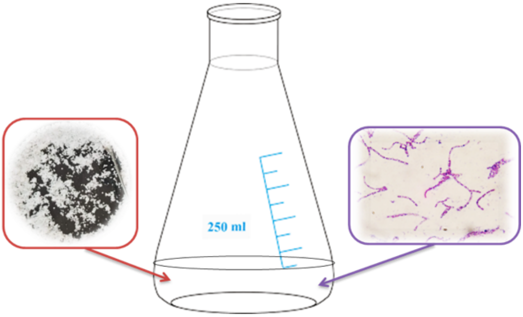
Microplastics, as a particles size <5 mm, are cause of concern due to ubiquity presence at environment [1]. There are a lot of processes that are investigated in the purpose to remove these particles from the environment, including the bioremediation [2]. In this study, biodegradation of polystyrene (PS) and polyvinyl chloride (PVC) by bacterium *Bacillus cereus* according to Taguchi design of experiments were investigated. Seven factors (pH-value, temperature, size of microplastic particles, concentration of microplastics, agitation speed, optical density of bacterial suspension, and addition of glucose) were investigated. According to the obtained results (increasing CFU) show that tested bacterial culture have the ability to degrade PS and PVC.



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P66 - Structure elucidation, Hirshfeld surface analysis, and Quantum computations of a thiazole derivative

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Thiazole is an important moiety in the field of heterocyclic chemistry. Thiazole derivatives display a wide spectrum of biological activities like antimicrobial, anticancer, anticonvulsant, antineoplastic, anti-inflammatory, antibacterial and antitumor.[1] The title compound Ethyl 5-(thiophene-2-carbonyl)thiazole-4-carboxylate was crystallized in the monoclinic crystal system with the space group P21/c. The asymmetric unit contains two independent molecules. The unit cell parameters are a = 8.1772(14) Å, b = 22.564(4) Å, c = 12.939(2) Å, and β = 95.154°. Hirshfeld surface analysis reveals the presence of intermolecular interactions in the crystal.[2] The DFT calculations were performed to analyze the frontier molecular orbitals (HOMO – LUMO) [2]. The Hirshfeld surface mapped over d_{norm} (a), and HOMO and LUMO of the molecule (b) are shown in figure 1, respectively.

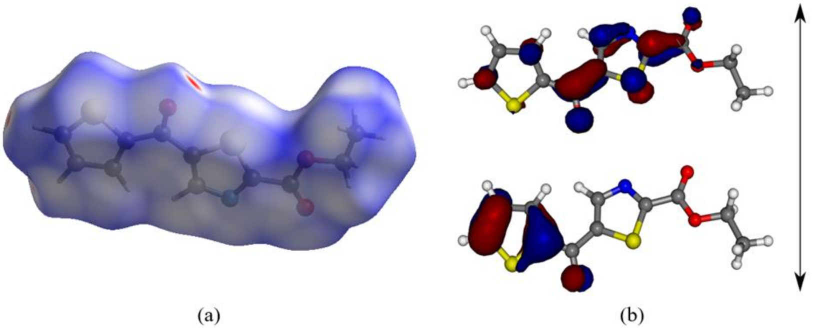

Figure 1. Hirshfeld surface mapped over d_{norm} (a), and HOMO and LUMO of the molecule (b)

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P67 - Effects of alloying on hot carrier generation

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Metal nanostructures have lately been a subject of extensive research due to useful properties of localized surface plasmons – coherent oscillations of conduction electrons – that such structures enable. When plasmons decay high energy charge carriers (*hot carriers*) are produced. Hot carriers can be used in photovoltaics, sensing and photocatalysis but there is little insight into how their energy distribution can be tuned [1]. In this work we use density functional theory (DFT) to explore the possibility of tuning the hot carrier energy distribution by alloying. Results are obtained by a method most commonly used in literature [2] which is compared to a method we propose as an alternative.

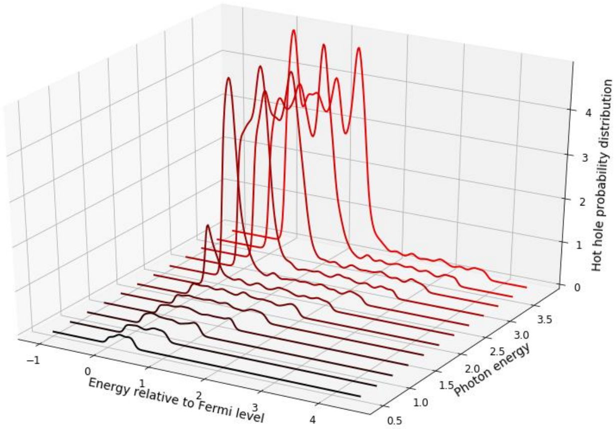

Figure 1 Initial hot electron generation probability distributions upon excitation with photons of different energies in copper-gold alloy system characterized by a fcc-like Cu_3Au unit cell.

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P68 - Corrosion and microhardness behavior of FeNiBSi metallic glass

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In general, FeNi-based metallic glasses are good soft magnets which have high potential for different applications due to their interesting and unique properties, especially excellent corrosion and mechanical properties [1].
Experimental results of corrosion and microhardness behavior of $Fe_{38}Ni_{36}B_{18}Si_8$ metallic glass alloy were presented and it was discussed how thermal treatment influences these properties. The alloy was produced by melt spinning technique and it was previously characterized comprehensively [2]. Some very recent results show that the thermal treatment influences corrosion properties of $Fe_{38}Ni_{36}B_{18}Si_8$ metallic glass alloy [3] so the alloy with very similar concentration was examined, but different thermal treatment. Additionally, metallographic investigation and microhardness measurements were performed.

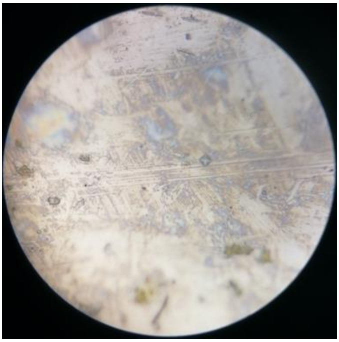

Figure 1 A print during microhardness measurement.

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P69 - Surface plasmons in Dirac/Weyl semimetals

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Three-dimensional topological Dirac/Weyl semimetals [1, 2], which can be seen as the three-dimensional analogs of graphene, have been intensively studied recently. The dielectric formalism within the random phase approximation (RPA) gives a bulk plasmon mode which is responsible for the appearance of a well-defined surface plasmon mode in the structure factor [3]. The obtained surface plasmon dispersion always stays below the bulk plasmon dispersion. In addition, Weyl semimetals comprise surface Fermi arc electron states which result with an anisotropic Fermi arc plasmon mode.

We study the modification of the surface plasmon mode due to the Fermi arc plasmon mode using the dielectric formalism [4] and the Bogoliubov transformation technique for a model Hamiltonian [5].The obtained results for the surface plasmon mode are consistent with the recent experimental data in these materials [6].

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P70 - *On a Novel Magnetoelectric Oxide Cu_4O_3*

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A laboratory preparation of paramelaconite (Cu_4O_3), a member of the group of natural minerals even more rare than diamond, is anything but a straightforward task [1]. In this work, a Cu_4O_3 phase stable up to, at least, 923 K was prepared via reduction of a copper(II) oxide. XRD and magnetic data agree well with those reported on the mineral sample [2], while magnetic susceptibility reveals an antiferromagnetic transition at 44.7 K, and two novel transitions at 70 K and 120 K. Electric conductivity was shown to depend on frequency, and yields a strong resonance feature at 36.52 kHz at RT. From electric conductivity and time relaxation measurements one can calculate a magnetic permittivity $\mu_r = 3790$ and dielectric permittivity $\varepsilon_r = 6{,}6 \cdot 10^6$. Calculation of electronic densities of states (DOS) provides the route to the Jahn-Teller (JT) distortion, as a precondition for the stress exerted onto the crystal lattice. Similar to other strong dielectric materials, a solely microscopic approach to the problem doesn't explain the huge dielectric permittivity. We applied a Maxwell-Wagner (MW) model which is based on the mesoscopic properties and puts forward an effect referred to the literature as internal grain boundary barrier layer capacitance (IBLC).In this work the IBLC model was supplemented by a viscoelastic contribution on the grain boundaries. Calculations, however, give the dielectric permittivity two orders of magnitude lower than measured. An application of the Dzyaloshinsky-Moriya ferromagnetic model and anisotropic magnetic superexchange do match the neutron scattering data [2]. The possible explanation for dielectric and magnetic properties resides on the Dirac-Weyl-Majorana fermions. In addition, electric resistance obeys the semimetallic properties, while spin-orbit interaction lifts a small degeneracy near Fermi level.

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[2] L. P. Gaudart, J. R. Carvajal, A. Gukasov, P. Monod, *Phys. Rev. B* **69** (2004) 104408.

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