Curriculum Vitae

1. Personal Information

Name: Javier Martí-Rujas

Place of birth: Tarragona, Spain.

Languages:, Catalan (mother tongue), Spanish, Italian, fluent spoken and English, fluent both spoken and written.

2005: PhD in Solid-State Chemistry from Cardiff University, Wales, (UK), (Prof. Kenneth D. M. Harris).

2006: Postdoc Department of Chemistry, Georgetown University, USA, (Prof. Jennifer A. Swift).

2007: Postdoc at Cardiff University Wales, UK in 2007-2008 (Prof. Kenneth D. M. Harris).

2008-2010: Japan Society for the Promotion of Science (JSPS) for Foreign Researchers fellowship at the Graduate School of Engineering of the University of Tokyo, Japan, (Prof. Makoto Fujita).

2010-2012: Senior Postdoc at Center for Nano Science and Technology at the Italian Institute of Technology in Milano, Italy.

2012-2017: Principal Investigator at the Center for Nano Science and Technology at the Italian Institute of Technology in Milano, Italy.

2017-2018: Adjunct lecturer, Faculty of Science, Universitat Autonoma de Barcelona, Spain.

2018-: Associate Professor at the Dipartimento di Chimica Materiali e Ingegneria Chimica "Giulio Natta", Politecnico di Milano, Italy.

2. Research Background

Summary of Research Background: My research interests are in the area of solid state chemistry of hybrid metal organic compounds and pure organic materials both at the fundamental and applied level. The goal of my research is to develop new structure-based functional materials. I am currently studying supramolecular structures that are self-assembled via **coordination bonds** and electrostatic forces through **second sphere coordination** interactions. Using coordination bonds, a new type of one-dimensional (1D) coordination polymers as host-guest systems has been synthesized and characterized using single crystal X-ray diffraction and *ab initio* X-ray powder diffraction techniques as the main tool. Using second-sphere interactions via hydrogen bonds, we have successfully synthesized a new hybrid metal organic material that displays racemic polymorphism and strong non-linear optical (NLO) properties. More recently, research towards the synthesis of perovskites focusing on lead-free perovskites (collaboration with Dr. Annamaria Petrozza's group the Istituto Italiano di Tecnologia) by means of second sphere interactions is attracting major attention in our group.

My strong expertise is in X-ray crystallography. I carry out structure elucidation of small molecules (organic and hybrid metal organic materials) using in-house X-ray diffractometers both single crystal and powder X-ray techniques. I am very interested in the use of **synchrotron** beam lines such as Spring-8 (Osaka) and Photon Factory (Tsukuba) both in Japan, PAL-POSTECH, (Pohang) South Korea and ALBA-CELLS (Barcelona), Spain, to study microcrystalline diffraction and poorly diffracting materials (*i.e.*, single crystal and powder materials). In

a collaborative work, I am applying the latest advances in Quantum Mechanics (Prof. Famulari, Politecnico di Milano) specific for solid-state systems to understand the reactivity and stability of all our newly synthesized materials. I am also interested in applying synthetic chemistry to develop new organic molecules that can be used as building blocks in the hybrid metal organic materials I am developing.

3. Research Accomplishments

1. Current Research and Further Goals.

Current Research.

Design and synthesis of new hybrid metal organic materials and structural aspects of organic co-crystals: The actual research that I am carrying out is focused in the rational design and synthesis of new functional organic and hybrid metal organic materials. The strategy is to use **coordination bonds** and **electrostatic interactions** (hydrogen bonds) to self-assembly metals with organic molecules to form hybrid metal organic materials containing open spaces or channels that can include guest molecules with the goal of giving new functional properties. Also, co-crystallization of organic materials including pharmaceutical materials are being investigated. Those studies are aimed at monitoring their structural stability, phase transformations and polymorphic behavior of the organic (pharmaceutical) compounds.

Coordination Polymers: New rod-like pyridine based organic ligands are being synthesized to construct new coordination polymers (CPs) (also known as Metal Organic Frameworks (MOFs)) by exploiting the labile nature of the coordination bonds. Through different crystallization methods such as slow diffusion, instant synthesis and solid liquid interface reaction, a variety of different crystalline materials with different properties are being obtained. Acting as filters, we are developing CPs that can adsorb small chlorinated volatile organic molecules (Cl-VOCs) such as chloroform, dichlormethane and dichloroethane, but also saturated and unsaturated alkanes, which can be stored for several weeks without being released to the atmosphere. Moreover the adsorption of Cl-VOCs seems selective (Chem. Comm., 2015; Dalton 2016). Exploiting the solid liquid interface method (Chem. Comm, 2010) we are able to synthesize the CP in good yields (96%), fast (5 mins) and using very small amount of solvent. It is our idea that these materials and crystallization methods can be exploited for many other new CPs (Dalton 2016). Also we discovered second harmonic generation (SHG) phenomena in a different CP which is obtained in the solid-state after a desolvation process (Dalton, 2015). This is important for potential applications in areas of photonics such as electro optics and frequency conversion. A combination of single crystal X-ray diffraction and *ab initio* X-ray powder diffraction techniques, including synchrotron data (ALBA-CELLS), have been used to elucidate the crystalline structures (Dalton 2015).

Hybrid Metal-Organic Second Sphere Adducts: In order to create new functional materials is necessary to exploit the properties that metal ions and organic cations together can give as a self-assembled entity. In this project, **second sphere coordination** (SSC) interactions are being used to create new functional hybrid metal organic materials (Cryst. Growth Des. 2014). Second-sphere coordination refers to any intermolecular interaction with the ligands directly bound to the primary coordination sphere of a metal ion. SSC hybrid materials are different from the above CPs as the interactions holding together the building blocks are electrostatic instead of coordination bonds. By means of crystal engineering principles we are tackling the synthesis of new lead-free, copper-based hybrid perovskite following a second-sphere coordination approach to obtain lead-free, copper-based hybrid perovskite following a second-sphere coordination approach with potential applications in solid-state lighting (ChemPlusChem, in Press, 2017; Highlighted in Front Cover and Cover Profile).

As defined by Gibb's Phase Rule, polymorphism refers to the situation in which two or more crystalline phases have the same chemical composition but different chemical structures. Usually polymorphism is confined to pharmaceutical organic materials but has not exploited in hybrid second sphere adducts. Using racemic crystals, we are exploiting the potential to observe polymorphism in second sphere adducts. Particularly, the aim of this research line is to attempt the **rational design of non-centrosymmetric materials** (Dalton 2015) which are at the core of the development of NLO materials for applications in electro-optics, frequency conversion, piezoelectricity and ferroelectricity. Recently, we have found a system which is polymorphic and one of the polymorphs is non-centrosymmetric and polar, and as a result shows significant SHG (CrystEngComm, 2016).

Exploiting SSC the ionic conductivity within 1D channels was reported and from a fundamental aspect, we are also interested in developing **solid-state mechanochemical reactions** to study the conversion of second sphere adducts to coordination complexes following dehydrochlorination reactions (CrystEngComm 2014; Hot Paper and Cover; Inorg. Chem. 2014).

In addition an active collaboration with Prof. A. Famulari at Politecnico di Milano, Quantum-mechanical calculations specific-for solid-state have been used to rationalize the observed X-ray structures and the reactivity of those materials upon external stimuli like mechanical forces, temperature, etc.

Synthesis, Structural Analysis and Thermal Stability in Organic and Pharmaceutical Co-crystals: Another research topic that I am interested is to study structural aspects of molecular salts and co-crystals and the interconversion depending on the stoichiometry. Using single crystal and powder X-ray diffraction, we described the reversible solid state ionic interconversion between A_1B_1 and A_1B_2•H_2O (where A = acid and B = base) and vice versa upon neat grinding by adding one equivalent of (B/A•2H_2O) respectively. This allows for the synthesis of co-crystals that in solution cannot be obtained but using the already formed co-crystal the synthesis can be done (CrystEngCom 2013, Cryst. Growth Des. 2014). In order to rationalize the experimental results and to gain insights on the role of water molecules in the formation of crystalline salts, the relative stabilities of the crystalline phases were compared by quantum mechanics calculations specific for solid state systems. This approach is being currently used to study pharmaceutic compounds.

Further Goals

Structural characterization of hybrid metal organic materials using single crystal diffraction and powder X-ray analysis to assess their potential function as nanoreactors.

The interest of our research is in the synthesis and preparation of hybrid metal organic materials (MOMs) to explore their functional properties in areas such as chemical separation, gas adsorption, ionic conductivity, NLO properties such as ferro- and piezoelectricity and solid-state luminescence. Currently we are exploiting a new crystallization method in CPs synthesis: the solid liquid interface method. This method is able to produce the desired material in short times, quantitative yields and in large quantities but as microcrystals. The crystalline structures are isostructural containing 1D channels with opening sizes about 7.5 Å × 8.9 Å (Chem. Comm., 2015). The size and chemical enviroment of the channels can be tunned by changing the halogens in the Zn salt used (Dalton 2016). By replacing the metal ions (Zn^{2+} for Mn^{2+}, Cu^{2+}, Fe^{2+}) we have obtained a variety of new CPs as microcrystalline powders which require the crystallographic analysis by ab initio X-ray powder diffraction (XRPD) using synchrotron radiation. From preliminary results, we have detected that one of our 1D CPs can trap linear hydrocarbons including alkanes, alkenes and alkines via single-crystal-to-single-crystal in a gas adsorption reaction. Although we have an initial single crystal structural analysis where we can see that the inclusion of the hydrocarbons occurs, a more elaborated structural characterization method using a combination of single crystal XRD (SCXRD) and ab initio XPRD analysis will be essential. The precise structural information, will be crucial to understand the exact position of the double and triple bonds in the guest molecules included in the 1D channels, and upon UV irradiation, depending on their relative positions within the 1D channels, might react to give unexpected new materials (i.e., by means of intermolecular [2+2] photocyclization reactions). Besides selectivity of branchend and linear alkanes which is of crucial importance in many industrial processes such as oil refining, our goal is also to use the 1D nanochannels as suitable reaction vessels to study solid-state polymerizaiton reactions within the CPs. First the studies will be on single crystals and later it will be expanded into microcrystals obtained via solid liquid interface to obtain large scale products. To begin with, monomers such as isoprene, pentadiene, acrylonitrile will be included in the channels via single-crystal-to-single-crystal following a gas-solid reaction. Upon monomer inclusion, gamma-ray-induced polymerization of the CPs including the monomers will be carried out to form regular polymers. It is know that some of the polymers such as polyacrylonitrile (PAN) is a semicrystalline resin, however the crystalline nature of the CPs can allow its single crystal X-ray elucidation if the

reaction does not degrade its single crystallinity. Structure elucidation both by SCXRD and ab initio XRPD analysis will be crucial for the deep understanding of the as synthesized materials, and of the products obtained via solid-state reactivity.

Development of hybrid lead-free halide perovskites for photovoltaics and solid-state lighting: Over the last four years, lead halide perovskites have been attracting major interest for applications in photovoltaic energy conversion, photodetection and light emission. In particular, light emitting devices (LEDs), field effect light-emitting transistors (LE-FETs) and tunable lasers were reported recently. However, most of these technologies rely heavily on Pb-based perovskites, such as methylammonium lead iodide ($MaPbI_3$) and cesium lead bromide ($CsPbBr_3$), and because of the toxicity and strict regulations of lead-based products, their commercialization could be strongly hampered. Therefore, for this reason, the development of alternative lead-free perovskites is needed. The future research I envisage is in the development of new lead-free perovskites by applying the rational design upon crystal engineering principles by means of electrostatic interactions. Although, crystal structure prediction is far from reaching desired levels of accuracy, it is still possible to plan, based on crystal engineering principles, the rational design of solid materials by combining building blocks via second-sphere coordination involving reversible hydrogen bonding interactions. The aim is to synthesize new perovskites that can be prepared as thin films and that incorporated in devices for applications in solid-state lighting and photovoltaic energy conversion.

Solid liquid interface method for the crystallization of coordination polymers: Another research topic that I would like to work is on the synthesis of new coordination polymers using solid liquid interface method. This method is still unexplored but offers the possibility to synthesize in large scale, short crystallization times and quantitative yields microcrystalline materials. These three aspects are crucial for the potential commercialization of a given coordination polymer and hence its successful industrial application. Clearly, although we have reported to cases of such non-conventional crystallization method (Chem. Comm., 2010; Dalton 2016), there is plenty of space to develop further and understand the conditions during the solid-liquid interface reaction allowing us to obtain the targeted material. Since crystallization is sometimes very difficult to control, the solid liquid interface method is definitely a new aspect in the crystallization are that needs to be explored. Due to the rapid crystallization conditions usually the new materials are kinetic products. In other words, the microcrystalline powders are metastable an can be transformed via external stimuli to more stable (thermodynamic) structures giving us the opportunity to explore functional materials that can be activated by external stimuli (*i.e.*, heat, light, pressure, etc).

Synthesis of discrete structures using halogen bonding for ion sensing: Halogen bonding (XB) is an emerging tool in the toolbox of any chemist and material scientist. About ten years ago XB was considered to be quite similar to hydrogen bonds, however during the last five years it has been demonstrated that it has distinctive features that make XB different from HB. The halogen bond is the noncovalent interaction in which halogen atoms behave as electrophilic species (electron density acceptors, Lewis acids). XB shows strong directionality.

While there have been many reports of halogen bonded adducts (i.e., co-crystals), there are not many examples of discrete structures such as bowls or cages self-assembled via XB displaying functional applications. By means of ligand design, our aim is to investigate the formation of discrete structures self-assembled using XB interactions, to create new materials featuring advanced physicochemical properties such as ion sensing (*i.e.*, particularly F^- anion) in a research area that still remains quite unexplored.

Polymorphic behavior in molecular solids pharmaceutical materials studied by combining *ab intio* XRPD and solid state NMR spectroscopy: In organic molecular solids, particularly in the pharmaceutical industry, is of crucial importance to understand the polymorphic behavior of a given drug. Particularly in the solid-state regarding its stability over time (*i.e.*, spontaneous transformation induced by dehydration or kinetic to thermodynamic transformation) at conditions in which the drugs are stored such as room temperature. The

evolution of a given drug might imply that the crystalline material is obtained as microcrystals and the structure elucidation has to be carried out using *ab initio* XRPD analysis.

In this project the aim is to combine solid-state NMR and computational simulation using DFT calculations (collaboration with Prof. Kenneth D.M. Harris, Cardiff University) with *ab initio* XRPD to elucidate the crystalline structure of microcrystalline materials (powders) that are not possible to be studied using single crystal X-ray diffraction. This approach is very powerful and provides a robust vindication of the correctness of the crystal structure by assessing the quality of agreement of the structure both with experimental powder X-ray diffraction data and with experimental solid-state ^{13}C NMR data.

2. Summary of Graduate and Postdoctoral Work.

Understanding the Molecular Transport and Reactivity in Organic Structures: During my PhD, I studied the *in situ* molecular transport of linear alkanes through one-dimensional tunnels in solid urea inclusion compounds using Confocal Raman Microspectrometry. Particularly, I studied fundamental aspects of this transport process (i.e., exchange of 1,8-dibromooctane for pentadecane guest molecules), focusing on the distribution of the guest molecules in the crystal and the changes in their spatial distribution as a function of time (JACS 2004, J. Phys. Chem, B, 2006). The data provided significant information about the conformational changes of guest molecules during the transport process, and allowed the design of a model to determine the rate of guest exchange (kinetics) (J. Phys. Chem B, 2007; J. Phys. Chem C, 2009).

I also carried out research on the solid state reactivity of organic molecules. Complete *ab initio* structure determination from powder X-ray diffraction of a polymeric material obtained directly from a solid state polymerization reaction, of 2,5-distyrylpyrazine (DSP) was carried out (J. Phys. Chem. C 2008). In this reaction, polymerization occurs by means of intermolecular [2 + 2] photocyclization reactions at each end of the monomer molecule. High-resolution solid-state ^{13}C NMR was used to confirm this reaction.

Kinetic Control and Structural Transformations in Coordination Networks: The kinetic control, thermodynamic stability and solid-state reactivity of isostructural 3D coordination networks were studied using *ab initio* powder X-ray diffraction. The coordination networks studied are kinetically-controlled interpenetrated open-frameworks that contain nitrobenzene guest molecules. We demonstrate that fast precipitation (i.e., instant synthesis) can selectively produce metastable networks that are not possible to synthesize by conventional solution chemistry (JACS 2009, JACS 2011). We provided mechanistic insights into thermally induced (573 - 723 K) (i.e., annealing method) structural transformations in porous coordination networks, as well as examples of guest exchange/inclusion reactions. The work had been highlighted in the **Research Frontiers** magazine published by **Spring-8** synchrotron facility. Moreover, using the kinetic effect in coordination networks, the selective inclusion of tetratiafulvalene (TTF) molecules showing very short S···S contacts was also demonstrated in an open framework containing two types of channels using synchrotron *ab intio* XRPD analysis (Angew. Chem. Int. Ed. 2011). The above research was published in Accounts of Chemical Research (Acc. Chem. Res. 2013).

Synthesis of Organic Open Frameworks via Supramolecular Chemistry: 1,6-Bis(trimethylammonium)hexane bis(trihalides) and mixed bis(trihalides) have been synthesized by treating the corresponding dihydrated halides with molecular dihalogens under gas–solid and solution conditions (CrystEngComm, 2011). Despite the starting halides being non-porous, the trihalide syntheses occur homogeneously, in quantitative yields, and reversibly. The stability of the obtained trihalides is mainly due to cooperative halogen bond and cation templating effect. Upon heating we also demonstrated the dynamic behavior and the solid state reactivity of 1,6-Bis(trimethylammonium)hexane bis(trihalides) and mixed bis(trihalides) were by releasing one molecule of I_2 the virtually unknown tetrahalide species $[I_4]^{2-}$, $[I_2Br_2]^{2-}$, and $[I_2Cl_2]^{2-}$ were formed (Angewandte Chem. Int. Ed. 2013; VIP Paper and Cover).

Applying crystal engineering principles, I carried out the self-assembly of an open framework by combining in an orthogonal way hydrogen and halogen bonds. Using a ligand with two pairs of sites for potentially orthogonal binding processes, simultaneous hydrogen bonding and halogen bonding was demonstrated to occur in a chemically and geometrically orthogonal manner. Indeed, the pure ligand in the crystal self-assembles by pairing the two couples of complementary binding sites, which are saturated via multiple halogen bonds. The two-dimensional network was able to sustain gas-solid guest exchange single-crystal-to-single-crystal reactions by exchanging dioxane for 1,3 dibromobenzene (Chem. Comm. 2012).

5. Publication List

1. Javier Martí-Rujas, Arnaud Desmedt, Kenneth D. M. Harris and François Guillaume

Direct time-resolved and spatially resolved monitoring of molecular transport in a crystalline nanochannel system.

J. Am. Chem. Soc., **2004**, *126*, 11124–11125.

2. Javier Martí-Rujas, Arnaud Desmedt, Kenneth D. M. Harris and François Guillaume

Significant conformational changes associated with molecular transport in a crystalline solid.

J. Phys. Chem. B, **2006**, *110*, 10708–10713.

3. Javier Martí-Rujas, Arnaud Desmedt, Kenneth D. M. Harris and François Guillaume

In-situ monitoring of alkane-alkane guest exchange in urea inclusion compounds using confocal Raman microspectrometry.

Mol. Cryst. Liq. Cryst., **2006**, *456*,139–147.

4. Javier Martí-Rujas, Arnaud Desmedt, Kenneth D. M. Harris and François Guillaume

Kinetics of molecular transport in a nanoporous crystal studied by confocal Raman microspectrometry: Single-file diffusion in a densely filled tunnel.

J. Phys. Chem. B, **2007**, *111*, 12339–12344.

5. Fang Guo, **Javier Martí-Rujas**, Zhigang Pan, Colan E. Hughes and Kenneth D. M. Harris

Direct structural understanding of a topochemical solid-state photopolymerization reaction.

J. Phys. Chem. C, **2008**, *112*, 19793–19796.

6. Javier Martí-Rujas, Arnaud Desmedt, Kenneth D. M. Harris and François Guillaume

Bidirectional transport of guest molecules through the nanoporous tunnel structure of a solid inclusion compound.

J. Phys. Chem. C, **2009**, *113*, 736–743.

7. Kazuaki Ohara, **Javier Martí-Rujas**, Tsuyoshi Haneda, Masaki Kawano, Daisuke Hashizume, Fujio Izumi and Makoto Fujita

Formation of thermally stable porous coordination networks via a crystalline-to-amorphous-to-crystalline phase transition.

J. Am. Chem. Soc., **2009**, *131*, 3860–3861.

8. Javier Martí-Rujas, Anabel Morte-Ródenas, Fang Guo, Nigel Thomas, Kotaro Fujii, Benson M. Kariuki and Kenneth D. M. Harris

A solid-state dehydration process in an organic material associated with substantial hydrogen-bond reorganization, investigated by powder X-Ray diffraction.

Cryst. Growth Des., **2010**, *10*, 3176–3181.

9. Javier Martí-Rujas, Yoshitaka Matsushita, Fujio Izumi, Makoto Fujita and Masaki Kawano

Solid-liquid interface synthesis of microcrystalline porous coordination networks.

Chem. Commun., **2010**, *46*, 6515–6517.

***10. Javier Martí-Rujas**, Nazrul Islam, Daisuke Hashizume, Fujio Izumi, Makoto Fujita and Masaki Kawano

Dramatic structural rearrangements in porous coordination networks

J. Am. Chem. Soc., **2011**, *133*, 5853–5860.

→"Highlighted Paper in Spring-8 Research Frontiers"

11. Marcos D. Garcia, **Javier Martí-Rujas**, Pierangelo Metrangolo, Carlos Peinador, Tullio Pilati Giuseppe Resnati and Giancarlo Terraneo

Dimensional caging of polyiodides: cation-templated synthesis using bipyridinium salts.

CrystEngComm. **2011***, 13,* 4411–4416.

12. Lorenzo Meazza, **Javier Martí-Rujas**, Pierangelo Metrangolo, Giancarlo Terraneo, and Giuseppe Resnati

Solid-State synthesis of mixed trihalides via reversible absorption of dihalogens by non poruous onium salts.

CrystEngComm. **2011***, 13,* 4427–4435.

13. Javier Martí-Rujas, Islam, Nazrul, Daisuke Hashizume, Fujio Izumi, Makoto Fujita and Masaki Kawano

Ab initio powder diffraction structure analysis of a host-guest network: Short contacts between tetrathiafulvalene molecules in a pore.

Angew. Chem. Int. Ed., **2011***, 50*, 6105–6108*.*

14. Javier Martí-Rujas, Benson M. Kariuki, Colan E. Hughes, Anabel Morte-Ródenas, Fang Guo, Zornita Glavcheva-Laleva, Kemal Taştemür, Li-ling Ooi, Lily Yeo and Kenneth D. M. Harris

Structural diversity, but not polymorphism, in a homologous family of co-crystals of urea and *α,ω*-dihydroxyalkanes.

New J. Chem., **2011**, *35,* 1515–1521.

15. Antonio Abate, **Javier Martí-Rujas**, Pierangelo Metrangolo, Tullio Pilati, Giuseppe Resnati and Giancarlo Terraneo

Tetrahedral oxyanions in halogen-bonded coordination networks.

Cryst. Growth Des., **2011**, *11*, 4220–4226.

16. Paolo Gondoni, Matteo. Ghidelli, Fabio Di Fonzo, Valeria Russo, Paola Bruno, **Javier Martí-Rujas**, Carlo Enrico Bottani, Andrea Li Bassi and Carlo Spartaco Casari

Structural and functional properties of Al:ZnO thin films grown by pulsed laser deposition at room temperature.

Thin Solid Films, **2012**, *520*, 4707–4711.

***17**. **Javier Martí-Rujas** and Masaki Kawano

Structural memory effect in solid-state transformation of kinetic coordination networks.

Spring-8 Research Frontiers, **2012**, 86-87.

→Research Highlights of 2011 at SPring-8

18. Javier Martí-Rujas, Luca Colombo, Jian Lü, Archan Dei, Giancarlo Terraneo, Pierangelo Metrangolo, Tullio Pilati and Giuseppe Resnati

Hydrogen and halogen bonding drive the orthogonal self-assembly of an organic framework possessing 2D channels

Chem. Commun., **2012**, *48*, 8207–8209.

19. Jingxiang Lin, **Javier Martí-Rujas**, Pierangelo Metrangolo, Tullio Pilati, Stefano Radice, Giuseppe Resnati and Giancarlo Terraneo

Solution and solid state synthesis of the discrete polyiodide I_7^{3-} under modular cation templation.

Cryst. Growth Des. **2012**, *12*, 5757–5762.

20. **Javier Martí-Rujas** and Masaki Kawano

Kinetic products in coordination networks: Ab initio X-Ray powder diffraction analysis.

Acc. Chem. Res., **2013,** *46*, 493–505.

21. Paolo Gondoni, Matteo. Ghidelli, Fabio Di Fonzo, Valeria Russo, Paola Bruno, **Javier Martí-Rujas**, Carlo Enrico Bottani, Andrea Li Bassi and Carlo Spartaco Casari

Highly performing Al:ZnO thin films grown by pulsed laser deposition at room temperature.

Nanosci. and Nanotechnol. Lett. **2013**, *5*, 484–486.

22. Fang Guo, Ming-Qian Zhang, Antonino Famulari and **Javier Martí-Rujas***

Solid state transformations in stoichiometric hydrogen bonded molecular salts: ionic interconversion and dehydration processes.

CrystEngComm. **2013**, *15*, 6237–6243.

***23**. **Javier Martí-Rujas**, Lorenzo Meazza, Gin Keat Lim, Giancarlo Terraneo, Tullio Pilati, Kenneth D. M. Harris, Pierangelo Metrangolo and Giuseppe Resnati

An adaptable and dynamically porous organic salt traps unique tetrahalide dianions*.

Angew. Chem. Int. Ed., **2013**, *52*, 13444–13448.

→Very Important Paper- VIP

→Featured Inside Cover

24. Luca Passoni, Farbod Ghods, Pablo Docampo, Agnese Abrusci, **Javier Marti-Rujas**, Matteo Ghidelli, Giorgio Divitini, Caterina Ducati, Maddalena Binda, Simone Guarnera, Andrea Li Bassi, Carlo S. Casari, Henry J. Snaith, Annamaria Petrozza and Fabio Di Fonzo.

Hyperbranched quasi-1D nanostructures for solid-state dye sensitized solar cells.

ACS Nano, **2013**, *7*, 10023–10031.

25**. Fang Guo, Hui-de Shao, Qi Yang, Antonino Famulari and **Javier Martí-Rujas

Mechanochemical dehydrochlorination and chelation reaction in the solid-state: from a molecular salt to a coordination complex.

CrystEngComm. **2014**, *16*, 969–973.

→Selected as HOT Paper

→Highlighted in Cover Picture

26. **Javier Martí-Rujas*** and Massimo Cametti

Synthesis of a novel hybrid metal organic salt and its solid-state transformation.

New J. Chem., **2014**, *38*, 1385–1388.

27. Tommaso Nicolini, Antonino Famulari, Teresa Gatti, **Javier Martí-Rujas**, Francesca Villafiorita-Monteleone, Eleonora V. Canesi, Francesco Meinardi, Chiara Botta, Emilio Parisini, Stefano Valdo Meille and Chiara Bertarelli

Structure-photoluminescence correlation for two crystalline polymorphs of a thiophene-phenylene co-oligomer with bulky terminal substituents.

J. Phys. Chem. Lett., **2014***, 5*, 2171–2176*.*

28. Hong-yu Guan, Zhen Wang, Antonino Famulari, Xu Wang, Fang Guo and **Javier Martí-Rujas***

Synthesis of chelating complexes through solid-state dehydrochlorination reactions via second-sphere coordination interaction with metal chlorides: a combined experimental – molecular modeling study.

Inorg. Chem. **2014**. *53*, 7438–7445.

29. Francesco Fumagalli, **Javier Martí-Rujas** and Fabio Di Fonzo

Room temperature deposition of high figure of merit Al-doped zinc oxide by pulsed-direct current magnetron sputtering: Influence of energetic negative ion bombardment on film's optoelectronic properties

Thin Solid Films, **2014**, *569,* 44–51*.*

30. Lei Li, Francesco Maddalena, Malena Oliveros, Mario Caironi, Fang Guo and **Javier Martí-Rujas***

A second sphere coordination adduct containing one-dimensional water/methanol channels: X-ray structures, thermal stability and single crystal impedance spectroscopy analysis.

CrystEngComm, **2014**, *16*, 10888–10892.

31. Hong-liang Liu, Yi-Fei Xie, Zhi-gang Pan, Antonino Famulari, Fang Guo, Zhongfu Zhou and **Javier Martí-Rujas***

Cyclic interconversion among molecular salts via neat grinding and related photoluminescence properties.

Cryst. Growth Des. **2014**, *14*, 6528−6536*.*

32. Fang Guo, Xu Wang, Hong-yu Guan, Hai-bin Yu, Lei Li, Shan-shan Chen, Antonino Famulari and **Javier Martí-Rujas***

Tuning the inclusion properties and solid-state reactivity of second sphere adducts using conformationally flexible bidentate ligands.

Cryst. Growth Des.*,* **2015***, 15,* 2842−2852*.*

33**. **Javier Martí-Rujas, Simone Bonafede, Dorearta Tushi and Massimo Cametti

Multiple single-crystal-to-single-crystal guest exchange in a dynamic 1D coordination polymer.

Chem. Commun., **2015**, *51,* 12357-12360.

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34. Hong-Cui Yu, Lei Li, Ji Gao, Jian Tong, Wenxu Zheng, Massimo Cametti, Antonino Famulari, Stefano Valdo Meille, Fang Guo* and **Javier Martí-Rujas***

Insights into the formation of chiral second sphere coordination complexes with aromatic tris amines: combined single crystal X-ray crystallography and molecular modeling analyses.

Dalton Trans., **2015**, *44*, 15960-15965.

35. P. Gondoni, P. Mazzolini, V. Russo, M. Diani, M. Amati, L. Gregoratti, V. De Renzi, G. C. Gazzadi, **Javier Martí-Rujas**, A. Li Bassi and C. S. Casari

Tuning electrical properties of hierarchically assembled Al-doped ZnO nanoforests by room temperature by pulsed laser deposition.

Thin Solid Films, **2015**, *594*, 12-17.

***36.** Daniele Mendola, Nidal Saleh, Nora Hellow, Nicolas Vanthuyne, Christian Roussel, Loïc Toupet, Franca Castiglione, Federica Melone, Tullio Caronna, Francesca Fontana, **Javier Martí-Rujas**, Emilio Parisini, Luciana Malpezzi, Andrea Mele and Jeanne Crassous

Synthesis and structural properties of Aza[*n*]helicene platinum complexes: control of *cis* and *trans* stereochemistry.

Inorganic Chemistry, **2016**, *55*, 2009-2017.

→Highlighted in Front Cover Picture

37. Massimo Cametti, Ilaria Bargigia and **Javier Martí-Rujas***

Dynamic single crystal to polycrystal transformation of a 1D-coordination polymer and its second harmonic generation.

Dalton Trans., **2016**, *45,* 1674-1678.

38. Lei Li, Jian Tong, Fang Guo and **Javier Martí-Rujas***

Crystal engineering of a hybrid metal-organic host framework and its single-crystal-to-single-crystal guest exchange using second sphere coordination.

CrystEngComm, **2016**, *18*, 2284-2288.

39. Francesco Tampieri, Letizia Colella, Ali Maghsoumi, **Javier Martí-Rujas**, Emilio Parisini, Matteo Tommasini, Chiara Bertarelli and Aantonio Barbon

Meeting the challenging electronic structure of thiophene-based heterophenoquinones.

J. Phys. Chem. C, **2016**, *120*, 5732-5740.

40. Hai-Bin Yu, Hai-Tao Li, Peng Zhang, Antonino Famulari, Fang Guo, Ilaria Bargigia and **Javier Martí-Rujas***

Exploiting polymorphism in second sphere coordination: thermal transformation, NLO properties and selective mechanochemical synthesis.

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41. Fang Guo and **Javier Martí-Rujas*** (Perspective Article)

Second sphere coordination of hybrid metal-organic materials: solid-state reactivity.

Dalton Trans., **2016**, 45, 13648-13662.

42. Massimo Cametti***** and **Javier Martí-Rujas***

Selective adsorption of chlorinated volatile organic compounds vapours by microcrystalline 1D coordination polymers.

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43. Daniele Cortecchia, Cesare Soci, Massimo Cametti, Aannamaria Petrozza,*** Javier Martí-Rujas***

Crystal engineering of a two-dimensional lead-free perovskite with functional Organic Cations by second sphere coordination.

ChemPlusChem, **2017**, 82, 681-685.

→Highlighted in Front Cover Picture;

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→Among Most Accessed articles during the period 05/2016 to 04/2017

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45. Hai Tao Li, Fang Guo*, Meng Kou, Antonino Famulari, Qiang Fu, **Javier Martí-Rujas***

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46. Fang Guo, Zhen Wang, Jin-Jing Zhang, Antonino Famulari, Hai-tao Li, **Javier Martí-Rujas***

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Dalton Trans., **2017,** *46,* 9466-9471.

47. Manuel Petroselli, Sara Mosca, **Javier Martí-Rujas**, Daniela Comelli and Massimo Cametti*

Mixed Staked Charge Transfer π-Organic Materials based on Anthracenyl Boronic Acid.

European Journal of Organic Chemistry, **2017**, 7190-7194.

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49. Ivana Pierro, Giorgia Zanchin, Emilio Parisini, **Javier Martí-Rujas**, Maurizio Canetti, Giovanni Ricci, Fabio Bertini, Giuseppe Leone

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Chem, Eur. J., **2018**, *24*, 19368-19372.

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CrystEngComm, **2018**, *20,* 6721-6726.

52. D. Cortecchia, S. Neutzner, J. Yin, T. Salim, A. R. Srimath Kandada, A. Bruno, Y. M. Lam, **J. Martí-Rujas**, A. Petrozza, C. Soci

Structure-controlled optical thermoresponse in Ruddlesden-Popper layered perovskites

APL Materials, **2018**, *6*, 114207.

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53. G. Leone, E. Groppo, G. Zanchin, G. A. Martino, A., Piovano, F. Bertini, J. Martí-Rujas, E. Parisini, G. Ricci.

Concerted Electron Transfer in Iminopyridine Chromium Complexes: Ligand Effects on the Polymerization of Various (Di)olefins

Organometallics, **2018**, 37, 4827-4840.

54. M. Ghirardello, S. Mosca, J. Marti-Rujas, L. Nardo, A. Burnstock, A. Nevin, M. Bondani, L. Toniolo, G. Valentini, D. Comelli.

Time-Resolved Photoluminescence Microscopy Combined with X-ray Analyses and Raman Spectroscopy Sheds Light on the Imperfect Synthesis of Historical Cadmium Pigments

Analitical Chemistry, **2018**, 90, 10771-10779.

55. G. Zanchin, I. Pierro, E. Parisini, J. Martí-Rujas, G. Ricci. G. Leone

Synthesis, structure and behavior of vanadium(III) diphosphine complexes in the homo- and co-polymerization of ethylene with norbornene: the ligand donor strength and bite angle make the difference

Journal of Organometallic Chemistry, **2018**, 861, 142-150.

56. H. Li, Y. Yang, A. Famulari, L. Xin, J. Martí-Rujas*, F. Guo*

Reactivity among first and second coordination spheres using a multiprotonated ligand and Cu(ii) in the solid-state

CrystEngComm, **2019**, 21, 4354-4362.

57. M. Cametti, Y. Sakata, J. Martí-Rujas, S. Akine

ON/OFF Control of the Flipping Motion of Diuranyl Bis(Salophen) Macrocycle by Extremely Strong Binding with Fluoride Ion

Inorg. Chem., **2019**, 58, 14871–14875.

58. M. Lippi, M. Cametti, J. Martí-Rujas

Ab initio powder X-ray diffraction structural analysis of bispidine based 1D coordination polymers: insights into their guest responsive behaviour

Dalton Trans., **2019**, 48, 16756-16763.

59. M. Kou, X. Zhai, W.-L. Duan, P. Zhang, **J. Martí-Rujas***, F. Guo,*

Exploring the sensing behavior in the detection of nitroaromatics using coordination complexes based on 4,4′-(1,3-phenylenedioxy)-dianiline ligand

Inorganica Chimica Acta., **2019**, 494, 154-159.

60. J. Martí-Rujas*

Thermal reactivity in metal organic materials (MOMs): From single-crystal-to-single-crystal reactions and beyond

Materials., **2019**, 12, 4088.

61. M. Lippi, J. Caputo, A. Famulari, A. Sacchetti, C. Castellano, F. Meneghetti, **J. Martí-Rujas**, M. Cametti.

Combined structural and theoretical investigation on differently substituted bispidine ligands: predicting the properties of their corresponding coordination polymers

Dalton Trans. **2020**, 49*,* 5965-5973.

62. S. Torresi, A. Famulari, **J. Martí-Rujas**,*

Kinetically Controlled Fast Crystallization of M12L8Poly-[n]-catenanes Using the 2,4,6-Tris(4-pyridyl)benzene Ligand and ZnCl2in an Aromatic Environment

J. Am. Chem. Soc., **2020**, 142*,* 9537-9543.

63. G. Colombo Dugoni, A., Baggioli, A. Famulari, A. Sacchetti, **J. Martí-Rujas**,* M. Mariani, E. Macerata, E. Mossini, A., Mele.

Structural properties of the chelating agent 2,6-bis(1-(3-hydroxypropyl)-1,2,3-triazol-4-yl)pyridine: A combined XRD and DFT structural study

RSC Advances **2020**, 10*,* 19629-19635.

64. M. Lippi, J. Caputo, F. Meneghetti, C. Castellano, **J. Martí-Rujas**,* M. Cametti*

Tuneable solvent adsorption and exchange by 1D bispidine-based Mn(ii) coordination polymersvialigand design

Dalton Trans. **2020**, 49*,* 13420-13429.

65. J. Martí-Rujas,* (Perspective Article)

Structural elucidation of microcrystalline MOFs from powder X-ray diffraction

Dalton Trans. **2020**, 49*,* 13897-13916.

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66. T. Gatti, F. Lamberti, **J. Martí-Rujas**, M. Zheng.

Thiophenes and Their Benzo Derivatives: Structure. (Book Chapter)

Reference Module in Chemistry, Molecular Sciences and Chemical Engineering **2020**.

doi.org/10.1016/B978-0-12-409547-2.14774-2

67. L. Catalano, L. S. Germann, P. Julien, M. Arhangelskis, I. Halasz, K. Užarević, M. Etter, R.E. Dinnebier, M. Ursini, M. Cametti, **J. Martí-Rujas**, T. Friščić, P. Metrangolo, G. Resnati, G. Terraneo

Open versus Interpenetrated: Switchable Supramolecular Trajectories in Mechanosynthesis of a Halogen-Bonded Borromean Network

Chem. **2021**, 7*,* 146-154.

6. Oral and Poster Presentations

1. Invited Lecture at The 3rd ICSU/IUPAC Workshop on Crystal Engineering. February 2017.

Invited Lecture: “Crystal Engineering of New Hybrid Metal Organic Materials for Adsoprtion of Volatile Molecules and their Solid-State Reactivity."

2. Invited Lecture at The 15th Meeting of the Asian Crystallographic Association (AsCA'16)”, Hanoi, Vietnam (2016).

Invited Lecture: “Selective Adsorption of Chlorinated Volatile Organic Compounds Vapours by Microcrystalline 1D Metal Organic Framework."

3. Invited Lecture at The 2015 International Chemical Congress of Pacific Basin Societies (Pacifichem), Honolulu, Hawaii, USA. (Dec 15-20, 2015).

Invited Lecture 1: “Exploring the Synthesis and Solid State Behavior of Coordination Polymers and Complexes"

Invited Lecture 2: “Exploring the Solid-state and Dynamic Behavior in Second Sphere Coordination Chemistry”

4. Invited Lecture Universita degli Studi di Padova, Padova, Italy. (Nov 2015).

Invited Lecture: “Multiple Single-Crystal-to-Single-Crystal Guest Exchange in a Dynamic 1D Coordination Polymer"

5. The 1st Japan-Italy Joint Symposium on Materials for Efficient Utilization of Elements. Palazzo Vendramin, Venice, Italy. (May 18th-19th -2014).

Invited Lecture: “Exploiting Second Sphere Coordination in the Design of Hybrid Metal Organic Salts (MOSs): from Solid State Reactivity to Ionic Conductivity"

6. The 12th Meeting of the Asian Crystallographic Association (AsCA'13). The Hong Kong University of Science and Technology (HKUST), Hong Kong. (December 7th-10th -2013).

Invited Lecture: “An adaptable and Dynamically Porous Organic Salt Traps Unique Tetrahalide Dianions”

7. Nata's Seeds Grow. From the crystallography and modelling of stereoregular polymers to the challenges of complex systems (November 21st-22nd of 2013). Milan. Italy.

Poster Title: “Mechanochemical Dehydrochlorination and Chelation Reaction in the Solid-State: From a Molecular Salt to a Coordination Complex”

8. International Conference on the Organic Solid State (ICCOSS- XXI). St Catherine's College, Oxford, UK (August 4th-9th -2013).

Poster Title: “An Adaptable and Dynamically Porous Organic Salt Traps Unique Tetrahalide Dianions”

9. IX Ciclo de Conferencias: Perspectivas de la Investigacion Quimica Actual. 6 November, La Coruna, 2012, Spain.

Invited Lecture: “Kinetic Products in Coordination Networks and its Ab Initio X-Ray Powder Diffraction Analysis”

10. Vth International Conference on Molecular Materials (MOLMAT 2012), 3-6 July, Barcelona, 2012, Spain.

Poster Title: “Hydrogen and Halogen Bonding Drive the Orthogonal Self-Assembly of a Purely Organic Framework Showing 2D Porosity”

11. International Union of Crystallography Meeting, Madrid 2011, Spain.

Lecture Title: “Solid-State Synthesis of Mixed Trihalides via Reversible Absorption of Dihalogens by Non-porous Onium Salts”

12. The 89th Annual Meeting of the Chemical Society of Japan, Nihon University, Tokyo. March 2009. Japan.

Lecture Title: “Dramatic Thermodynamic Rearrangement of a Crystalline Coordination Network via an Amorphous Phase“

13. International Conference on the Organic Solid State (ICCOSS-XVII). University of California, Los Angeles. July-2005. USA.

Lecture Title: “Exploring Molecular Transport Processes in Solid Organic Tunnel Structures”