Structural Dynamics Research Group

HEAD:

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GROUP MEMBERS:

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RESEARCH PROFILE:

Our research interests oscillate between Chemistry, Physics and Materials Science. They include: photocrystallography and solid-state structural dynamics, solid-state spectroscopy, chemical and physical crystallography for materials science, accurate crystallography under ambient and extreme conditions, computational chemistry, instrumentation and software development, crystal engineering.

CURRENT RESEARCH ACTIVITIES:

- Tracing of excited-state species in crystals and solution

Polynuclear transition-metal complexes often exhibit interesting optoelectronic or magnetic properties. The aim of our research is to deeply investigate the dynamics of light-induced processes, which occur both in crystals and in solutions. We focus our attention on charge transfer processes taking place in chemical systems containing multicentre coinage metal complexes and also in bridged transition metal complexes L_nM_1–bridge–M_2L_m (M_1, M_2 = Fe, Co, Cu, *etc*., bridge = CN, SCN, *etc*.; L_n, L_m = ligands). We are interested in finding relationships between molecular structure of such compounds, their configuration and charge distribution, metal-metal interactions and metal centre's communication through different linking groups, *etc*., and the macroscopic properties of the respective substances.

- Synthesis and characterisation of new photoswitchable materials

Currently, one of the main goals of chemistry and physics is to develop new materials that are able to respond rapidly and reliably to changes in local environment, and send out signals which let us know what is happening. Consequently, our research is dedicated to thorough and systematic investigations of the

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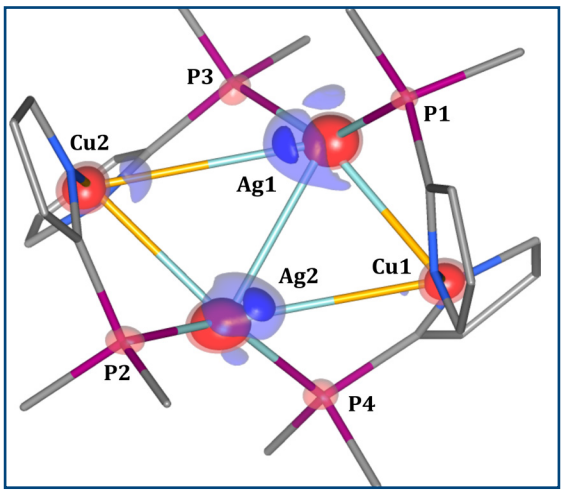
dynamics and nature of light-induced nitro group isomerisation reaction occurring in crystals of Ni, Cu or Co coordination compounds. We aim at designing promising photoswitchable materials characterised by desired reversibility, conversion percentage and stability.

- Crystal engineering

Crystal engineering methods are useful when analysing molecular motifs, relative crystal stabilities and origins of different properties of crystalline materials. We apply these tools to supplement our photocrystallographic studies and also to investigate crystals and cocrystals of boron-based compounds, pharmaceuticals and luminescent complexes, which have been of our interest for several years now.

- Method development and non-standard crystallography

Our scientific interests also cover preparation of useful tools (computer -codes, computational methods) and construction of devices for various crystallographic applications, including photocrystallography, experimental charge density studies and high-pressure crystallography. More details can be found on our website: **www.photocrystallography.eu**.



Photodifference map showing light-induced structural changes in a model silver(I)-copper(I) tetranuclear complex (reproduced from Inorg. Chem. 53 (2014) 10594).

SELECTED PUBLICATIONS:

1. D. Szarejko, R. Kamiński, P. Łaski, K.N. Jarzembska, Seed-skewness algorithm for X-ray diffraction signal detection in the time-resolved synchrotron Laue photocrystallography, J. Synchrotron Rad. (2020) 405.
2. S.E. Kutniewska, R. Kamiński, W. Buchowicz, K.N. Jarzembska, Photo- and thermoswitchable half-sandwich nickel(II) complex: [Ni(η^5-C_5H_5)(IMes)(η^1-NO_2)], Inorg. Chem. (2019) 16712.
3. K.N. Jarzembska, M. Hapka, R. Kamiński, W. Bury, S.E. Kutniewska, D. Szarejko, M.M. Szczęśniak, On the nature of luminescence thermochromism of multinuclear copper(I) benzoate complexes in the crystalline state, Crystals. 9 (2019) 36.
4. K.N. Jarzembska, R. Kamiński, K.F. Dziubek, M. Citroni, D. Paliwoda, K. Durka, S. Fanetti, R. Bini, Impact of high pressure on metallophilic interactions and its consequences for spectroscopic properties of a model tetranuclear silver(I)-copper(I) complex in the solid state, Inorg. Chem. 57 (2018) 8509.
5. K.N. Jarzembska, R. Kamiński. K. Durka, M. Kubsik, K. Nawara, E. Witkowska, M. Wiloch, S. Luliński, J. Waluk, I. Głowacki, K. Woźniak, New class of easily-synthesisable and modifiable organic materials for applications in luminescent devices, Dyes Pigm. 138 (2017) 267.
6. R. Kamiński, K.N. Jarzembska, S.E. Kutyła, M. Kamiński, A portable light-delivery device for in situ photocrystallographic experiments at home laboratory, J. Appl. Cryst. 49 (2016) 1383.
7. C.F.A. Negre, K.J. Young, M. Belén Oviedo, L.J. Allen, C.G. Sánchez, K.N. Jarzembska, J.B. Benedict, R.H. Crabtree, P. Coppens, G.W. Brudvig, V.S. Batista, Photoelectrochemical hole injection revealed in polyoxotitanate nanocrystals functionalized with organic adsorbates, J. Am. Chem. Soc. 136 (2014) 16420.
8. K.N. Jarzembska, A.A. Hoser, R. Kamiński, A.Ø. Madsen, K. Durka, K. Woźniak, Combined experimental and computational studies of pyrazinamide and nicotinamide in the context of crystal engineering and thermodynamics, Cryst Growth Des. 14 (2014) 3453.
9. K.N. Jarzembska, Y. Chen, J. Nasca, E. Trzop, D.F. Watson, P. Coppens, Relating structure and photoelectrochemical properties: electron injection by structurally and theoretically characterized transition metal-doped phenanthroline-polioxotitanate nanoparticles, Phys. Chem. Chem. Phys. 16 (2014) 15792.
10. K.N. Jarzembska, R. Kamiński, B. Fournier, E. Trzop, J.D. Sokolow, R. Henning, Y. Chen, P. Coppens, Shedding light on the photochemistry of coinage-metal phosphorescent materials: a time-resolved Laue diffraction study of an Ag^I-Cu^I tetranuclear complex, Inorg. Chem. 53 (2014) 10594.