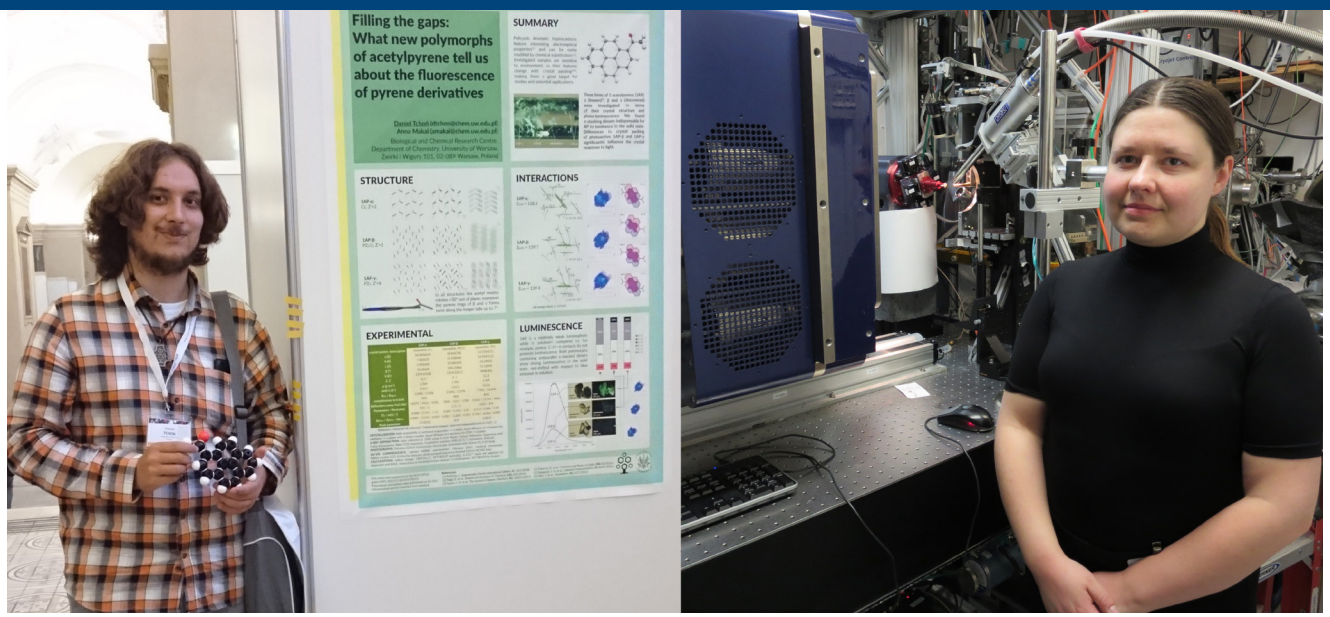
Structure – Function Analysis Group



HEAD:

Anna Makal*, PhD DSc

GROUP MEMBERS:

Roman Gajda, PhD
PhD student: Daniel Tchoń
BSc student: Aleksandra Zwolenik

RESEARCH PROFILE:

Application of crystallographic methods to describe how macroscopic physicochemical properties of solid materials depend on their microscopic crystal structure; specifically molecular environment, degree of ordering, presence of modulations and other factors. The methods include X-ray and neutron diffraction (single crystal and powder) under ambient and non-ambient conditions, quantum crystallography tools and periodic DFT calculations.

CURRENT RESEARCH ACTIVITIES:

Our current research concentrates on model luminescent compounds such as pyrene derivatives and gold (I) complexes and how modification of their crystalline environment affects their luminescence by inducing color change, enhancing or quenching it. Investigation of the relationship between the crystal structure, electron density distribution and (photo) physical properties of such materials is achieved by means of X-ray diffraction experiments performed both *in-house* and at the synchrotron facilities, UV-VIS spectroscopy and theoretical calculations.
Modifications of crystalline surroundings are achieved by applying variable temperature or pressure on a crystal as well as by growing new polymorphs. Obtaining a broad spectrum of polymorphs and solvates of a given substrate means that we have to handle metastable or unstable crystal forms and often work with incomplete or otherwise challenging datasets. For instance, a vast majority of organic and metalorganic

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luminescent compounds crystallize in low-symmetry systems, which makes them particularly challenging when performing experiments at non-ambient conditions. Optimization of high pressure X-ray diffraction experiments for low symmetry systems and predicting attainable data completeness is one of our current objectives. Software package enabling it is in preparation.
Unlike in conventional crystal structure determination, we enjoy studying all cases of disorder, modulation or chemical short range ordering which manifest themselves in non-Bragg intensities.

Fig. 1. (left) Cover for "Crystal morphology fixed by interplay of π-stacking and hydrogen bonds – the case of 1-hydroxypyrene", CrystEngComm, 2019, 21, 1701–1717; (middle) Anna Makal, Daniel Tchoń and Roman Gajda at a manuscript writing bootcamp, Kruszyniany, July 2019; (right) Cover for "The Impact of Crystal Packing and Aurophilic Interactions on the Luminescence Properties in Polymorphs and Solvate of Aroylacetylide–Gold(I) Complexes", Chem. Eur. J. 2019, 25, 13131–13145

SELECTED PUBLICATIONS:

1. M. Głodek, S. Pawlędzio, A. Makal, D. Plażuk, The Impact of Crystal Packing and Aurophilic Interactions on the Luminescence Properties in Polymorphs and Solvate of Aroylacetylide–Gold(I) Complexes, Chem. Eur. J. 25 (2019) 13131–13145.
2. D. Tchoń, D. Trzybiński, A. Wrona-Piotrowicz, A. Makal, Polymorphism and resulting luminescence properties of 1-acetylpyrene, CrystEngComm. 21 (2019) 5845–5852.
3. D. Tchoń, A. Makal, Structure and piezochromism of pyrene-1-carbaldehyde at high pressure, Acta Cryst. B75 (2019) 343–353.
4. R. Gajda, M.A. Domański, M. Malińska, A. Makal, Crystal morphology fixed by interplay of π-stacking and hydrogen bonds – the case of 1-hydroxypyrene, CrystEngComm. 21 (2019) 1701–1717.
5. A. Makal, J. Krzeszczakowska, R. Gajda, Pressure-Dependent Structural and Luminescence Properties of 1-(Pyren-1-yl)but-2-yn-1-one, Molecules. 24 (2019) 1107.
6. M. Głodek, A. Makal, P. Paluch, M. Kądziołka-Gaweł, Y. Kobayashi, J. Zakrzewski, D. Plażuk, (Ar–CO–C≡C)(PEt3)Au and (Ar–C≡C)(PEt3)Au complexes bearing pyrenyl and ferrocenyl groups: synthesis, structure, and luminescence properties, Dalton Transactions. 47(19) (2018) 6702–6712.
7. R. Flamholc, A. Wrona-Piotrowicz, A. Makal, J. Zakrzewski, Pyrenylpyrazole-based donor/acceptor fluorescent dyes: Synthesis and photophysical properties, Dyes and Pigments. 154 (2018) 52–61.
8. A. Makal, Triethylphosphine as a molecular gear — phase transitions in ferrocenyl–acetylide–gold(I), Acta. Cryst. B74 (2018) 427–435.