

# Daniel Mariusz Tchoń | CV

Institute of Physics of the Czech Academy of Sciences

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## Education

### Ph.D. in Chemistry

*Faculty of Chemistry, University of Warsaw*

Thesis "Polymorphism and luminescence of acetylated pyrene derivatives: analysis of structure and interactions based on single-crystal X-ray diffraction under pressure"

**Warsaw, Poland**

X 2017 – IX 2022

### M.Sc. in Chemistry

*Inter-faculty MISMaP College, University of Warsaw*

Thesis "Structural and charge density analysis of doxycycline based on high-resolution X-ray and neutron diffraction", with distinction

**Warsaw, Poland**

X 2015 – VI 2017

### B.Sc. in Chemistry

*Inter-faculty MISMaP College, University of Warsaw*

Thesis "Analysis of charge density in a popular antibiotic – doxycycline"

**Warsaw, Poland**

X 2012 – VII 2015

### Secondary education

*XIV High-school of Stanisław Staszic in Warsaw,*

„Mathematics and natural sciences" class profile with distinction each year

**Warsaw, Poland**

IX 2009 – V 2012

## Employment

### Postdoctoral Researcher

*Structure Analysis Dept., Institute of Physics, Czech Academy of Sciences*  
MSCA COFUND P4F postdoctoral researcher in the group of Dr. Lukáš Palatinus

- Developing software and methodology for Serial Precession Electron Diffraction

**Prague, Czechia**

XI 2024 –

### Postdoctoral Scholar

*MBIB, Biosciences Area, Lawrence Berkeley National Laboratory*

Crystallography specialist in the group of Dr. Nicholas Sauter

- Collecting and processing diffraction data from X-ray Free Electron Lasers
- Developing CCTBX software suite and accompanying modules

**Berkeley, CA, USA**

IX 2022 – IX 2024

### Junior Investigator

*Faculty of Chemistry, University of Warsaw*

Project "Local crystal and magnetic structure modelling in potential quantum spin liquid  $\alpha$ -RuCl<sub>3</sub>" under the supervision of PD Dr. Wojciech Sławiński

- Preparing, performing, and analyzing results of Single-Crystal X-Ray Diffraction (SCXRD) experiments of complex systems

**Warsaw, Poland**

X 2021 – III 2022

### Subcontracted Investigator

*Faculty of Chemistry, University of Warsaw*

Project "Experimental charge densities and structural studies of minerals - feasibility study" under the supervision of Prof. Krzysztof Woźniak

- Preparing, performing, and analyzing results of High-Pressure (HP) SCXRD experiments
- Participating in synchrotron HP SCXRD measurements and evaluating their results
- Teaching junior investigators methodology behind HP SCXRD techniques

**Warsaw, Poland**

VII 2020 – III 2021

## Junior Investigator

Faculty of Chemistry, University of Warsaw

Project "Structure and photophysical properties of selected pyrene derivatives in high pressure conditions" under the supervision of PD Dr. Anna Makal

- Preparing, performing, and analyzing results of HP SCXRD experiments, UV-Vis spectroscopic measurements, and periodic DFT calculations in ambient- and high-pressure conditions
- Participating in synchrotron HP SCXRD measurements and evaluating their results
- Writing scientific articles and presenting at international conferences

Warsaw, Poland

II 2016 – VIII 2019

## Intern

Diamond Light Source, Harwell Science & Innovation Campus

Beamline I19, under the supervision of Dr. Dave Allan and Dr. Mark Warren

- Preparing, performing, and analyzing results of HP SCXRD experiments
- Evaluating methodology of multi-crystal HP SCXRD measurements

Didcot, United Kingdom

VII 2017 – IX 2017

## Volunteer teacher

XIV High School in Warsaw

Organiser of extra-curricular chemistry classes, workshops, and laboratories

Warsaw, Poland

IX 2012 – VI 2019

Most of the volunteering and employment before 2022 was performed alongside education. Any apparent career breaks in this section are times when I focused primarily on my academic development.

## Publications

- Qiaoling, F., Willson, M. C., Foell, A. K., Paley, D. W., Kotei, P. A., Schriber, E. A., Rosenberg, D. J., Rani, K., Tchoń, D. M., Zeller, M., Melendrez, C., Kang, J., Inoue, I., Owada, S., Tono, K., Sugahara, M., Brewster, A. S. & Hohman, J. N. Nucleophilic Displacement Reactions of Silver-Based Metal–Organic Chalcogenolates. *J. Am. Chem. Soc.* **146**, 30349–30360 (2024).
- Blaschke, J. P., Bolotovskiy, R., Brewster, A. S., Donatelli, J., DuJardin, A., Feng, W., Ganapati, V., Kroeger, W., Mendez, D., McCorquodale, P., Mirchandaney, S., O'Grady, C. P., Paley, D. W., Perazzo, A., Poitevin, F. P., Poon, B. K., Ramakrishnaiah, V. B., Sauter, N. K., Shah, N., Slaughter, E., Sweeney, C., Tchoń, D., Uervirojnangkoorn, M., Wittwer, F., Wall, M. E., Yoon, C. H. & Young, I. D. ExaFEL: extreme-scale real-time data processing for X-ray free electron laser science. *Front. high perform. comput.* **2** (2024).
- Jastrzębska, R., Poręba, T., Cova, F., Tchoń, D. M. & Makal, A. Structure–property relationship of a complex photoluminescent arylacetylide-gold(I) compound. I: a pressure-induced phase transformation caught in the act. *IUCrJ* **11**, 737–743 (2024).
- Zwolenik, A., Tchoń, D. & Makal, A. Evolution of structure and spectroscopic properties of a new 1,3-diacetylpyrene polymorph with temperature and pressure. *IUCrJ* **11**, 519–527 (2024).
- Łomzik, M., Błaż, A., Tchoń, D., Makal, A., Rychlik, B. & Plazuk, D. Development of Half-Sandwich Ru, Os, Rh, and Ir Complexes Bearing the Pyridine-2-ylmethanimine Bidentate Ligand Derived from 7-Chloroquinazolin-4(3H)-one with Enhanced Antiproliferative Activity. *ACS Omega* **9**, 18224–18237 (2024).
- Ganapati, V., Tchoń, D., Brewster, A. S. & Sauter, N. K. Self-Supervised Deep Learning for Model Correction in the Computational Crystallography Toolbox. *arXiv* **2307**, 01901 (2023).
- Łomzik, M., Błaż, A., Głodek, M., Makal, A., Tchoń, D., Ayine-Tora, D. M., Hartinger, C., Rychlik, B. & Plazuk, D. Organometallic Ru, Os, Rh and Ir half-sandwich conjugates of ispinosib – impact of the organometallic group on the antimetabolic activity. *Dalton Trans.* **52**, 11859–11874 (2023).
- Gajda, R., Tchoń, D. & Makal, A. Hierarchy of Intermolecular Interactions in Highly Luminescent Pyrenyl-Pyrazole-Aldehyde. *Cryst. Growth Des.* **23**, 862–872 (2023).

- Gajda, R., Piekara, A., Tchoń, D., Woźniak, K. & Sławiński, W. Charge density studies of single and transient (single to double) Boron-Oxygen bonds in  $(NH_4)_2B_4O_5(OH)_4 \cdot 2H_2O$ . *Dalton Trans.* **51**, 14865-14874 (2022).
- Trzybiński, D., Wróbel, A., Tchoń, D., Kelland, M. A. & Woźniak, K. Structural studies of halide hexaalkylguanidinium salts. *J. Mol. Struct.* **1265**, 133338 (2022).
- Tchoń, D. & Makal, A. Maximizing completeness in single-crystal high-pressure diffraction experiments: phase transitions in 2°AP. *IUCrJ* **8**, 1006–1017 (2021).
- Tchoń, D., Bowskill, D., Sugden, I., Piotrowski, P. & Makal, A. Three new polymorphs of 1,8-diacetylpyrene: a material with packing-dependent luminescence properties and a testbed for crystal structure prediction. *J. Mater. Chem. C* **9**, 2491–2503 (2021).
- Łomzik, M., Hanif, M., Budniok, A., Błaż, A., Makal, A., Tchoń, D., Leśniewska, B., Tong, K. K. H., Movassaghi, S., Söhnle, T., Jamieson, S. M. F., Zafar, A., Reynisson, J., Rychlik, B., Hartinger, C. G. & Plažuk, D. Metal-Dependent Cytotoxic and Kinesin Spindle Protein Inhibitory Activity of Ru, Os, Rh, and Ir Half-Sandwich Complexes of Ispinesib-Derived Ligands. *Inorg. Chem.* **59**, 14879–14890 (2020).
- Tchoń, D., Trzybiński, D., Wrona-Piotrowicz, A. & Makal, A. Polymorphism and resulting luminescence properties of 1-acetylpyrene. *CrystEngComm* **21**, 5845–5852 (2019).
- Tchoń, D. & Makal, A. Structure and piezochromism of pyrene-1-carbaldehyde at high pressure, *Acta Cryst. B* **75**, 343–353 (2019).
- Tchoń, D., Makal, A., Gutmann, M. & Woźniak, K. Doxycycline hydrate and doxycycline hydrochloride dihydrate – crystal structure and charge density analysis. *Z. Kristallogr. Cryst. Mater.* **233**, 649–661 (2018).

## Notable dissemination activities

<b>11th Meeting of the German Young Crystallographers</b> <i>Oral and poster presentation</i>	<b>Neu-Isenberg, Germany</b> X 2024
<b>74th American Crystallographic Association Meeting</b> <i>Oral and poster presentation</i>	<b>Denver, Colorado, USA</b> VII 2024
<b>1st Meeting of the Polish Young Crystallographers</b> <i>Organisation support</i>	<b>Wrocław, Poland</b> VI 2022
<b>32nd Conference of the German Crystallographic Society</b> <i>Poster presentation</i>	<b>Bayreuth, Germany</b> III 2023
<b>73rd American Crystallographic Association Meeting</b> <i>Oral presentation</i>	<b>Baltimore, Maryland, USA</b> VII 2023
<b>33rd European Crystallographic Meeting</b> <i>Poster presentation</i>	<b>Versailles, France</b> VIII 2022
<b>63rd Polish Crystallographic Meeting</b> <i>Poster presentation</i>	<b>Wrocław, Poland</b> VI 2022
<b>2nd Virtual Scientific Conference of Ochota Campus</b> <i>Poster presentation</i>	<b>Warsaw, Poland</b> IX 2021
<b>25th Congress of the International Union of Crystallography</b> <i>Poster presentation</i>	<b>Prague, Czechia</b> VI 2021
<b>62nd Polish Crystallographic Meeting</b> <i>Oral and poster presentation</i>	<b>Wrocław, Poland</b> VI 2021

<b>1st Virtual Scientific Conference of Ochota Campus</b> <i>Poster presentation</i>	<b>Warsaw, Poland</b> <i>VI 2020</i>
<b>Joint Polish-German Crystallographic Meeting</b> <i>Oral and poster presentation</i>	<b>Wrocław, Poland</b> <i>II 2020</i>
<b>32nd European Crystallographic Meeting</b> <i>Poster presentation</i>	<b>Vienna, Austria</b> <i>VIII 2019</i>
<b>61st Polish Crystallographic Meeting</b> <i>Poster presentation</i>	<b>Wrocław, Poland</b> <i>VI 2019</i>
<b>HERCULES 2019 School</b> <i>Poster presentation</i>	<b>Grenoble, France</b> <i>III-IV 2019</i>
<b>European XFEL Users' Meeting 2019</b> <i>Poster presentation</i>	<b>Hamburg, Germany</b> <i>II 2019</i>
<b>HERCULES Regional School</b> <i>Poster presentation</i>	<b>Kraków, Poland</b> <i>XII 2018</i>
<b>56th European High Pressure Research Group Meeting</b> <i>Poster presentation</i>	<b>Aveiro, Portugal</b> <i>IX 2018</i>
<b>1st Conference of "Young Chemist's University"</b> <i>Main organizer</i>	<b>Warsaw, Poland</b> <i>VII 2018</i>
<b>60th Polish Crystallographic Meeting</b> <i>Poster presentation</i>	<b>Warsaw, Poland</b> <i>VI 2018</i>
<b>International School of Crystallography - 52nd Course: Quantum Cryst.</b> <i>Oral and poster presentation</i>	<b>Erice, Italy</b> <i>VI 2018</i>
<b>CM1402 Crystallize COST Meeting</b> <i>Passive participation</i>	<b>Praga, Czechia</b> <i>II 2018</i>
<b>4th European Crystallographic School</b> <i>Poster presentation</i>	<b>Warsaw, Poland</b> <i>VII 2017</i>
<b>59th Polish Crystallographic Meeting</b> <i>Poster presentation</i>	<b>Wrocław, Poland</b> <i>VI 2017</i>
<b>7th European Charge Density Meeting</b> <i>Organisation support, passive participation</i>	<b>Warsaw, Poland</b> <i>VI 2016</i>
<b>58th Polish Crystallographic Meeting</b> <i>Passive participation</i>	<b>Wrocław, Poland</b> <i>VI 2016</i>
<b>57th Polish Crystallographic Meeting</b> <i>Poster presentation</i>	<b>Wrocław, Poland</b> <i>VI 2015</i>
<b>MultiPole-2</b> <i>Passive participation</i>	<b>Warsaw, Poland</b> <i>V 2015</i>

## Notable research activities

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<b>SPring-8 Angstrom Compact Free Electron Laser</b> <i>Beamline 3, night shift SFX data processing lead</i>	<b>Kōto, Hyōgo, Japan</b> <i>IV 2024</i>
<b>Linac Coherent Light Source</b> <i>Hutch 4.5, MFX day shift SFX data processing support</i>	<b>Menlo Park, CA, USA</b> <i>III 2024</i>
<b>SPring-8 Angstrom Compact Free Electron Laser</b> <i>Beamline 3, night shift SFX data processing lead</i>	<b>Kōto, Hyōgo, Japan</b> <i>II 2024</i>
<b>Advanced Light Source</b> <i>Beamline 12.2.2, night shift XRD overall lead</i>	<b>Berkeley, CA, USA</b> <i>XI 2023</i>

<b>Linac Coherent Light Source</b> <i>Hutch 4.5 MFX, one-day SFX data processing support</i>	<b>Menlo Park, CA, USA</b> <i>XII 2022</i>
<b>Faculty of Chemistry and Pharmacy, University of Regensburg</b> <i>Study under Dr. Florian Kleemiss, implementing PDF display in Olex2</i>	<b>Regensburg, Germany</b> <i>VII 2022</i>
<b>Elettra Sincrotrone Trieste</b> <i>Beamline 11.2R Xpress, day shift XRD sample preparation and processing</i>	<b>Trieste, Italy</b> <i>XI 2021</i>
<b>SOLEIL Synchrotron Facility</b> <i>Beamline CRISTAL, overall XRD experiment support</i>	<b>Saint-Aubin, France</b> <i>IX 2021</i>
<b>Super Photon Ring – 8 GeV</b> <i>Beamline 02B1, day shift XRD sample preparation lead</i>	<b>Kōto, Hyōgo, Japan</b> <i>VI 2019</i>
<b>Diamond Light Source</b> <i>Beamline I19.2, 1-person XRD sample prep., data collection, processing</i>	<b>Didcot, United Kingdom</b> <i>VIII 2017</i>
<b>ISIS Neutron and Muon Source</b> <i>SXD instrument, neutron diffraction data processing support</i>	<b>Didcot, United Kingdom</b> <i>IX 2015</i>

## Notable contributions & awards

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- Presenting author on 14 international and 9 polish conferences, including 6 oral presentations
- Former user of neutron and photon sources including listed above and others (ANKA, SLS, ILL)
- Crystallographic software author: hikari, picometer, pRuby, DTools.pl; contributor: CCTBX, DIALS
- Member of the Polish (since 2022) and American (2023–2024) Crystallographic Associations
- Founding Member, Deputy Manager of Polish Young Crystallographers (2022, 2023, 2024 terms)
- Co-organizer, co-author of the 4th, 5th & 6th biennial Polish Crystallography Olympiad (2021–2025)
- Best Poster awardee at 62nd Polish Crystallographic Meeting, Second Virtual Scientific Conference of Ochota Campus, 74th American Crystallographic Association Meeting.
- Participant of Higher European Research Course for Users of Large Experimental Systems, 2019
- Participant of International School of Crystallography: Quantum Crystallography in Erice, 2018
- Organizer of "Young Chemist's University" offering 120 internships for high-school students, 2018
- 5th Place Laureate, 2nd Polish Crystallography Olympiad for M.Sc. students in June 2017
- Volunteer teacher working with the top-ranked Warsaw High Schools since 2012
- 16th Place Laureate, 58th Polish Chemistry Olympiad in April 2012.

## Other Skills

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**English:** Proficient (CEFR level C2, IELTS 8.5)

**Polish:** Proficient (mother tongue)

**Japanese:** Intermediate (CEFR level B1)

**German:** Elementary (CEFR level A2)

**IT:** Proficiency with Python 3,  $\LaTeX$ , Git, Unix, Windows, macOS  
Familiarity with Django, gnuplot, Rlang, C++, html & many others

**Teaching:** Licensed High School/Univeristy chemistry teacher

**Personal:** Stellar track of various leadership and organizational skills

