



# Sylwia Pawlędzio

## Chemist



12 October 1990



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## About me

Self-motivated chemistry graduate with experience in the scientific environment, teaching and publishing, closely working on active pharmaceutical ingredients and organometallic compounds and developing skills in a progressive scientific project which requires quantum crystallography expertise.

## Skills

Linux and Windows

Python

communication

problem-solving

team-working

flexible

English★5 Spanish★2 Russian★1

(\*)[The skill scale is from 0 (Fundamental Awareness) to 6 (Expert).]

## Experience

07.2023-ongoing Postdoctoral Research Fellowship

Oak Ridge National Laboratory

- *Mechanistic investigation of direct air capture with single-crystal neutron diffraction*

11.2022-04.2023 Research Scientist

University of Warsaw

Contractor in grant:

- *Phase transitions in minerals induced by pressure and studied by experimental charge densities - feasibility studies (Opus, NCN, 2019-ongoing)*

2015-2022 Ph.D. study

University of Warsaw

Managed four scientific projects:

- *Application of quantum crystallography methods to detect relativistic effects in crystal structures with heavy elements (Preludium, NCN, 2019-2021);*
- *Hirshfeld Atom Refinement taking into account the relativistic effects of heavy atoms (DSM, MSWiA, 2018-2019);*
- *High-resolution X-ray diffraction experiments of acridine derivatives (DSM, MSWiA, 2017-2018);*
- *Preparation, structure and properties of new co-crystals of carbamazepine and benzoic acid derivatives (DSM, MSWiA, 2016-2017).*

Contractor in grants:

- *Advancing quantum crystallography for better insight into structure and properties of crystals (Opus, NCN, 2019-ongoing)*
- *TEAM-TECH project "Core facility for crystallographic and biophysical research to support the development of medicinal products" (TEAM TECH CORE FACILITY, Foundation for Polish Science, 2017-2019)*
- *Structure and distribution of the electron density in crystals as a source of information on the interactions of pharmaceutical substances (Maestro, NCN, 2015-2018)*

The most important knowledge:

- In-depth analysis of relationship between crystal structure and electron density distribution in crystals
- Knowledge of crystallization techniques
- Structure solution and refinement (IAM, multipolar model, HAR, XCW fitting, TAAM)
- Data analysis and manuscript preparation
- Quantum mechanical calculations in solid state studies
- Continuous work with the Protein Data Bank and Cambridge Structural Database
- Performing X-ray diffraction experiments using in-house equipment as well as synchrotron radiation facility with applying high pressure or low temperature
- Ability to work with several chemical programs: *Olex2, Mercury, WinGX, Tonto, XD2016, MoPro, Platon, CrysAlisPro, Apex3, Mole-QoolQT, Discamb, NoSpherA2, Orca, Gaussian, Crystal*
- Results evaluation and presentation during international conferences, workshops and schools
- Supporting, educating and supervising students

## Education

- 2015–2022 Ph.D. candidate in Chemistry University of Warsaw  
*Application of quantum crystallography methods for the detection of relativistic effects and description of aurophilic interactions for model crystal structures with heavy atoms, pass with distinction*
- 2014–2015 M.Sc. in Chemistry University of Warsaw  
*Structures and electron density of ferrocene taxol analogues*
- 2009–2014 B.Sc. in Chemistry University of Warsaw  
*Polymorphic structures of glycine*

## Awards and scholarships

- 2022
- IUCr Young Scientists Awards – travel grant to attend 33<sup>rd</sup> European Crystallographic Meeting, Versailles, France
  - Young Scientist Bursary covering conference fee of 9<sup>th</sup> International Charge Density Meeting, Aarhus, Denmark
- 2021
- IUCr Young Scientists Awards – accommodation grant to attend IUCr 2021 XXV General Assembly and Congress of the International Union of Crystallography, Prague, Czech Republic
  - Bursary covering conference fee of IUCr2021 – Electron crystallography satellite school, Prague, Czech Republic
  - UW Rector Scholarships given for the 10% best students in 2021/2022
  - Increase in Doctoral Scholarship given for the 30% best students in 2021/2022
- 2020
- UW Rector Scholarships given for the 10% best students in 2020/2021
  - Increase in Doctoral Scholarship given for the 30% best students in 2020/2021
  - The University's Integrated Development Programme ZIP Fellowship
- 2019
- Best Poster Presentation during International Charge Density Meeting, Göttingen, Germany
  - IUCr Young Scientists Awards – travel grant to attend 32<sup>nd</sup> European Crystallographic Meeting, Vienna, Austria
  - Increase in Doctoral Scholarship given for the 30% best students in 2019/2020
- 2018
- Scholarship for accommodation cost during International School of Crystallography – Quantum Crystallography Course, Erice, Italy
  - Scholarship to attend *Crystallize COST Action Meeting*, Prague, Czech Republic
- 2017
- IUCr Young Scientists Awards – travel grant to attend School on Charge Density and MoPro, Mexico City, Mexico
  - IUCr Young Scientists Awards – accommodation grant to attend International School of Biological Crystallisation, Granada, Spain

## Conferences

2022

- 33<sup>rd</sup> European Crystallographic Meeting, Versailles, France, poster presentation
- 9<sup>th</sup> International Charge Density Meeting, Aarhus, Denmark, poster presentation

2021

- IUCr 2021 XXV General Assembly and Congress of the International Union of Crystallography, Prague, Czech Republic, oral presentation
- 29<sup>th</sup> Annual Meeting of German Crystallographic Society, Online Meeting, Hamburg, Germany, oral presentation

2020

- Quantum Crystallography Online Meeting, Paris, France, poster presentation
- Joint Polish-German Crystallographic Meeting, Wrocław, Poland, oral presentation

2019

- 32<sup>nd</sup> European Crystallographic Meeting, Vienna, Austria, poster presentation
- International Charge Density Meeting, Göttingen, Germany, poster presentation

2018

- 31<sup>st</sup> European Crystallographic Meeting, Oviedo, Spain, poster presentation
- 7<sup>th</sup> Intercollegiate Biotechnology Symposium *Symbioza*, Warsaw, Poland, poster presentation
- General meeting of an international research network *COST Action Meeting*, Prague, Czech Republic, poster presentation

2016

- 7<sup>th</sup> European Charge Density Meeting, Warsaw, Poland, poster presentation
- 58 *Konwersatorium Krystalograficzne*, Wrocław, Poland, poster presentation
- 7<sup>th</sup> Seminar of Ph.D. Students in Chemists - *ChemSession'16*, Warsaw, Poland, poster presentation
- 59<sup>th</sup> Scientific Conference for Students of Physics and Natural Sciences *Open Readings 2016*, Vilnius, Lithuania, poster presentation

2015

- National Student Conference *NMD VI - "Nowoczesne metody doświadczalne w fizyce, chemii i inżynierii"*, Lublin, Poland, oral presentation
- International Conference *Multipole2 - "Multi-Pole Approach to Structural Science"*, Warsaw, Poland, poster presentation

## Internships and scientific trips

2022

- Short-term scientific trip to SLS synchrotron station in Villigen, Switzerland

2021

- Short-term scientific trip to SOLEIL synchrotron station in Saint-Aubin, France

2020

- Short-term internship in prof. Simon Grabowsky's Research Group, Universität Bern, Bern, Switzerland

2019

- Short-term scientific trip to The Advanced Photon Source (APS) synchrotron station in Chicago, USA
- Short-term scientific trip to the SPring-8 synchrotron station in Sayo, Japan

2018

- Short-term internship in prof. Simon Grabowsky's Research Group, Universität Bremen, Bremen, Germany

## Schools and Workshops

2021

- IUCr2021 – Electron crystallography satellite school, Prague, Czech Republic

2018

- *HERCULES-SOLARIS* Regional School, Cracow, Poland
- International School of Crystallography – Quantum Crystallography Course, Erice, Italy

2017

- 4<sup>th</sup> European Crystallography School, Warsaw, Poland
- School on Charge Density and MoPro, Mexico City, Mexico
- International School of Biological Crystallization, Granada, Spain

2016

- International School of Crystallization, Granada, Spain

## Interests

Research

X-ray and electron diffraction, experimental charge density, topological analysis of the electron density, intermolecular interactions (hydrogen bonds, aurophilic interactions), metal-organic compounds, polymorphism, quantum crystallography, relativistic effects

General

reading non-fiction literature, understanding cultural diversity, volunteering at scientific picnics, traveling, stretching, acro pole dance