

Call for Applications for a PhD Student Position

Project: Dynamic Quantum Crystallography for Better Understanding Thermodynamic Stability and Solubility of Drug Cocrystals

Location: Faculty of Chemistry, University of Warsaw

Project leader: dr hab. Anna Hoser

Finansowanie: SONATA BIS 15

The research group of dr. hab. Anna Hoser, at the Faculty of Chemistry, University of Warsaw, is seeking a PhD student to work on the SONATA BIS project entitled “Dynamic Quantum Crystallography for Better Understanding Thermodynamic Stability and Solubility of Drug Cocrystals.”

The project focuses on the experimental and computational investigation of the solubility of pharmaceutical cocrystals. Cocrystallization is one of the approaches used to modify and enhance the solubility of active pharmaceutical ingredients (APIs). The aim of the project is to synthesize a range of cocrystals of selected APIs and experimentally determine and compare their solubilities. Their crystal structures will then be investigated using single-crystal X-ray diffraction or electron diffraction. The experimental results will be correlated with results obtained using quantum crystallography, in particular through NoMoRe refinements.

The research conducted by the group combines crystallography with quantum-chemical calculations. The group develops new methods for the rapid estimation of vibrational entropy and, consequently, for predicting the relative stability of polymorphs and cocrystals. One of the methods being developed is the refinement of normal-mode frequencies against single-crystal X-ray diffraction data, known as NoMoRe (nomore.chem.uw.edu.pl). The resulting frequencies are used to calculate thermodynamic properties, including heat capacity and vibrational entropy, and to assess crystal stability.

Main duties:

- Synthesis of cocrystal
- Structural characterization of cocrystals via single-crystal X-ray (SC-XRD) and 3D electron diffraction (3D-ED)
- Cocrystal solubility measurements
- Involvement in the preparation of scientific publications
- Presentation of results at international conferences
- Supervision of students.

Specific Requirements:

- A master's degree (or equivalent) in chemistry awarded before the position's start date
- Good written and verbal communication skills in English.
- Practical experience in synthesis and crystallisation (cocrystals, polymorphs) and mechanochemistry
- Practical experience in single crystal X-ray diffraction (SCXRD) data collection and structure solution.
- ability to work effectively both independently and as part of a team

Additional assets:

- experience in “Normal Mode Refinement (NoMoRe)”

The candidate must meet the requirements specified in art. 113 of the Act of 20 July 2018 – Law on Higher Education and Science (Journal of Laws of 2018, 1668, as amended).

Benefits:

- A full-time PhD scholarship for 48 months, amounting to PLN 5,000 net per month for candidates admitted to the Doctoral School through the standard recruitment process in June. In the case of recruitment outside the standard admission process, the scholarship may be significantly lower and amount to PLN 5,000 gross per month.

Required documents:

- A detailed CV
- A cover letter outlining research experience, career goals, and specific interest in this position.
- Information on personal data processing (available for download at:
<http://www.chem.uw.edu.pl/oferty-pracy/>)

Please submit the documents by 20th of September 2026 to email: a.hoser@uw.edu.pl, with “PhD position” in the subject line. The results of the competition will be given by e-mail no later than 14 days after the competition has been concluded.