



UNIVERSITY
OF WARSAW



Doctoral School of
Exact and Natural
Sciences

Competition notice

PRELUDIUM BIS

Project title: **Computational design of magnetic metal-organic frameworks using ab initio crystal structure prediction**

Research project manager: dr hab. Mihails Arhangelskis

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Project description:

In the Arhangelskis group we develop methods for the computational design of crystalline materials with the aim of improving the speed and reducing the costs of materials development, while also driving our understanding of structure-property relationships.

Our major research interest is in the development of crystal structure prediction (CSP) of metal-organic frameworks (MOFs), which are functional materials constructed from transition metal nodes connected by organic linkers. MOFs are renowned for the diversity of functional applications, including gas storage, catalysis, materials for energy storage, magnetic materials and many more. The diversity of functional properties arises from the vast number of possible combinations of nodes and linkers, each leading to materials with different crystal structures and, consequently, functional properties. Design of new MOFs, therefore, requires extensive experimental screening of node and linker combinations, in a quest to find materials, showing desired functional properties.

The CSP method, developed in our group,¹ provides an alternative approach to MOF design from a computational perspective: starting from a 2D diagram of nodes and linkers we are able to predict which crystal structures are most likely to form from experimentally, and then simulate the functional properties of the predicted structures. In particular, we have recently applied this method to the design of MOFs with potential application as rocket fuels.²

The current PhD project is dedicated to the application of CSP to the design of magnetic MOF materials. In these materials, the transition metal atoms with unpaired electrons carry magnetic moment, however, it is the organic linkers that allow to control the distance between magnetic centers and their orientation, thereby influencing the overall magnetic performance.³ Our objective is to reliably predict structures of MOFs that possess strong magnetic performance at possibly higher temperatures.

The successful candidate will use state-of-the art computational methods, namely periodic density-functional theory (DFT) calculations and machine learning (ML) to predict the crystal structures and magnetic properties (magnetic ordering, Curie temperature) of putative MOF structures.

The studentship also includes a 6-month internship (supported by NAWA) with Dr. Krunoslav Užarević at the Ruđer Bošković Institute (Zagreb, Croatia), where the candidate will receive training in the experimental synthesis and characterization of MOF materials, including magnet measurements.

To enquire about the project please email m.arhangelskis@uw.edu.pl. For further information about the Arhangelskis group please visit the group website www.arhangelskis.org

References

- (1) Darby, J. P.; Arhangelskis, M.; Katsenis, A. D.; Marrett, J. M.; Frišćić, T.; Morris, A. J. *Chem. Mater.* **2020**, *32*, 5835–5844.
- (2) Xu, Y.; Marrett, J. M.; Titi, H. M.; Darby, J. P.; Morris, A. J.; Frišćić, T.; Arhangelskis, M. *J. Am. Chem. Soc.* **2023**, *145*, 3515–3525..
- (3) Muratović, S.; Martinez, V.; Karadeniz, B.; Pajić, D.; Brekalo, I.; Arhangelskis, M.; Mazaj, M.; Mali, G.; Etter, M.; Frišćić, T.; Krupskaya, Y.; Kataev, V.; Žilić, D.; Užarević, K. *Inorg. Chem.* **2022**, *61*, 18181–18192.

Requirement

The call is open to all those who are not PhD holders and are not students at the doctoral schools.

- Masters degree in chemistry, materials science or related fields.
- Experience with quantum chemical calculations (periodic DFT would be advantageous).
- Good command of spoken and written English.

Optional skills:

- Ability to measure and process X-ray diffraction data.
- Experience with various solid-state characterization techniques, e. g. solid-state NMR, magnetic measurements, thermal analysis.

Discipline: chemical sciences

Admission limit: 1

Recruitment schedule

- registration in the Internet Registration of Candidates, referred to as “IRK”, submitting an application to the IRK: from 10 May to 09 June 2023
- qualification procedure: from 14 June to 23 June 2023
- announcement of the ranking list: until 30 June 2023
- accepting documents from qualified candidates: from 3 July to 21 September 2023

– announcement of the list of accepted candidates: until 30 September 2023

Beginning of education – October, 2023.

Recruitment fee

200 PLN

Form of the qualification proceedings

Qualification proceedings include the assessment of the following items:

- 1) the candidate's scientific activity, based on their CV or Resume, documented by scans of materials attached to the application for admission to the School;
- 2) an interview with the candidate;
- 3) other achievements.

Language of the selection process, including the interview

The interview shall be carried out in Polish or English – in accordance with the candidate's preferences presented in IRK. If the Polish language is selected, the interview may include parts in English.

Required documents

The candidate shall submit a School admission application only through the IRK. The application shall include the following:

- 1) indication of the selected discipline in which the candidate plans to pursue education or in the case of applying for the Interdisciplinary Doctoral School – fields of science with the specification of the leading field (and where there is no leading field – at least two equivalent disciplines), PESEL number or passport number, nationality, contact information (residence address, e-mail address, telephone number), information whether the candidate agrees to receive administrative decisions by means of electronic communication, consent for processing of personal data for the purposes of the admissions procedure;
- 2) a scan of the graduation diploma of uniform master's degree or postgraduate studies or an equivalent diploma obtained under separate regulations or in the case of candidates pursuing education within the European Higher Education Area – a certificate of obtaining a Master's degree or a declaration that the diploma or certificate of obtaining a Master's degree shall be provided by 21.09.2023 – declaration form. In case the diploma was issued in a language other than Polish or English, the candidate shall attach its certified translation;
- 3) a resume or CV outlining the candidate's scientific activity, including scholarly interests and achievements during the five calendar years preceding the application (if a candidate became a parent during this time, as evidenced by a scan of the child's birth certificate attached to the application, this period shall be extended by two years for each child), including, but not limited to:
 - publications,
 - research and organizational work at student research groups,
 - participation in scientific conferences,
 - participation in research projects,
 - awards and honorable mentions,
 - research internships,

- research skills training programs completed,
 - activities promoting science,
 - activity in science movement representative bodies,
 - average of their university grades,
 - professional career,
 - level of proficiency in foreign languages;
- 4) scans of materials evidencing scientific activity mentioned in their CV and/or resume;
 - 5) a document confirming at least B2 proficiency level in English or a declaration of the level of proficiency in English allowing education at the School;
 - 6) the scan of a declaration by the planned supervisor, confirming their agreement to undertake the duties of a supervisor and of the number of doctoral students, for whom they perform the duties a designated supervisor, in accordance with the template constituting Appendix no.4 to the Resolution no. 17 of the Senate of the University of Warsaw of 20th January 2021 on rules of admission to doctoral schools at the University of Warsaw (the University of Warsaw Monitor of 2023, item 43), the candidate may also attach a scan of their planned supervisor's opinion and opinions of other academics about the candidate and their scientific activity and/or proposed research project;
 - 7) the photograph of a candidate's face that allows for their identification;
 - 8) a declaration confirming whether the candidate was or is a doctoral student or a participant of doctoral studies or whether they have initiated a doctoral dissertation process or whether proceedings to award them a doctoral degree have been initiated – and if yes, the title of their doctoral dissertation or the research project prepared by a candidate, including the name and last name of the candidate's tutor or supervisor;
 - 9) a declaration confirming that they have reviewed the Resolution no. 17 of the Senate of the University of Warsaw of 20th January 2021 on rules of admission to doctoral schools at the University of Warsaw (the University of Warsaw Monitor of 2023, item 43) and Articles 40 and 41 of the Code of Administrative Procedure;
 - 10) scanned transcripts of records of the graduate and postgraduate studies or the uniform Master's degree studies, or equivalent documents (e.g. diploma supplement);
 - 11) abstract of the master's thesis or master's project in English (up to 3,000 characters with spaces);

Evaluation criteria

- a) competencies to perform specific tasks in a research project (70% of the final score)
 - 3 points - very good
 - 2 points – good
 - 1 point – poor
 - 0 points - no competencies
- b) publication track record, including publications in renowned scientific papers / magazines (30% of the final score)
 - 4 points – prominent
 - 3 points - very good
 - 2 points – good
 - 1 point – poor
 - 0 points - no publication track record

Education program

The education lasts 4 years. It includes obligatory classes (no more than 300 hours in total during the whole period of education) and the implementation of an individual research program, carried out under the supervision of a supervisor. Beginning of education – October 1, 2023.

Scholarships

PRELUDIUM BIS doctoral scholarships shall amount to:

- PLN 4266.00 gross per month, until the month in which a PhD student's mid-term evaluation is performed at the doctoral school and
- PLN 5119.00 gross per month, after the month in which a PhD student's mid-term evaluation is performed at the doctoral school and

shall be awarded pursuant to the Act on Higher Education and Science of 20 July 2018.