UNIWERSYTET WARSZAWSKI
Wydział Chemii

Warsaw (Poland) 18/07/2024

Offer of a PhD studentship

Position of a **PhD student** in the project "**Computational design of next generation rocket fuels based on hypergolic metal-organic frameworks**" financed by **National Science Centre (NCN)** is open for applications. The successful candidate will be supervised by Dr. Mihails Arhangelskis, becoming a member of the computational materials design group at the Faculty of Chemistry, University of Warsaw. More information about the group can be found on the website www.arhangelskis.org.

Project leader: **dr hab. Mihails Arhangelskis**

Grant number: **2023/51/B/ST5/01555**

Available positions: 1.

Project description
The aim of the project is the computational design of hypergolic metal-organic frameworks (MOFs), as the next generation solid rocket fuel materials that are rapidly ignitable upon contact with an oxidizer. This is achieved by using organic linkers that contain unsaturated double- and triple bond substituents, so-called trigger groups. Yet, there is ample evidence that hypergolic performance of MOFs strongly depends on the choice of metal nodes and overall crystal packing. The method of crystal structure prediction (CSP) allows us to explore the intricate relationships between node and linker composition, crystal structure and resulting MOF properties.

We have recently reported the first computational design of hypergolic MOFs using CSP, demonstrating the wide opportunities presented by this approach. Thanks to CSP we can now perform computational screening of MOF structures and reliably select candidate structures with interesting properties for experimental synthesis.

The PhD student will perform computational screening of hypergolic MOFs, where both node and linker types will be varied, in a quest to find materials with enhanced performance, that makes them worthy of experimental synthesis. Major focus will also be placed on enhancing the computational efficiency of the CSP calculations by bringing in methods for faster energy ranking of predicted structures through the use of machine-learnt potentials (MLPs).

The successful candidate will work in a multidisciplinary team and will be engaged in the development of computationally efficient methods for crystal structure and property prediction of hypergolic MOFs. The work will involve the use of quantum-mechanical methods, particularly periodic density-functional theory (DFT) calculations and machine learning (ML) methods.

ul. Ludwika Pasteura 1, 02-093 Warszawa
tel.: 22 55 26211 (biuro dziekana), faks: 22 55 26428
e-mail: dziekan@chem.uw.edu.pl, www.chem.uw.edu.pl

The research activities will proceed in close collaboration with our international colleagues, Prof. Tomislav Friščić and Dr. Andrew Morris (University of Birmingham).

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) Xu, Y.; Marrett, J. M.; Titi, H. M.; Darby, J. P.; Morris, A. J.; Friščić, T.; Arhangelskis, M. Experimentally Validated Ab Initio Crystal Structure Prediction of Novel Metal–Organic Framework Materials. *J. Am. Chem. Soc.* **2023**, *145*, 3515–3525.

(2) Titi, H. M.; Marrett, J. M.; Dayaker, G.; Arhangelskis, M.; Mottillo, C.; Morris, A. J.; Rachiero, G. P.; Friščić, T.; Rogers, R. D. Hypergolic Zeolitic Imidazolate Frameworks (ZIFs) as next-Generation Solid Fuels: Unlocking the Latent Energetic Behavior of ZIFs. *Sci. Adv.* **2019**, *5*, eaav9044.

(3) Darby, J. P.; Arhangelskis, M.; Katsenis, A. D.; Marrett, J. M.; Friščić, T.; Morris, A. J. *Ab Initio* Prediction of Metal-Organic Framework Structures. *Chem. Mater.* **2020**, *32*, 5835–5844.

(4) Xu, Y.; Chodkiewicz, M. L.; Woińska, M.; Trzybiński, D.; Brekalo, I.; Topić, F.; Woźniak, K.; Arhangelskis, M. Hirshfeld Atom Refinement of Metal–Organic Frameworks for Accurate Positioning of Hydrogen Atoms and Disorder Analysis. *Chem. Commun.* **2023**, *59*, 8799–8802.

(5) Arhangelskis, M.; Katsenis, A. D.; Morris, A. J.; Friščić, T. Computational Evaluation of Metal Pentazolate Frameworks: Inorganic Analogues of Azolate Metal–Organic Frameworks. *Chem. Sci.* **2018**, *9*, 3367–3375.

Necessary qualifications:

- MSc degree in chemistry, materials science or related fields
- Experience with quantum chemical calculations
- Good command of spoken and written English

Additional skills which would be advantageous:

- Experience with periodic DFT calculations or other methods of modelling structures of crystalline materials
- Experience with machine learning techniques

The candidate must meet the requirements of art. 113 of the Act - Law on Higher Education and Science dated July 20, 2018 (Journal of Laws of 2018, item 1668).

We offer:
a temporary 48 month contract with the University of Warsaw. The successful candidate will receive a stipend of 5000 PLN/month for the first 24 month of the project, which will be increased to 5340,90 PLN/month after mid-term evaluation.

There is also a possibility to receive additional stipend from the University of Warsaw Doctoral School of Exact and Natural Sciences. The nearest possibility to apply for this stipend will be June 2025, i. e. for the 2nd-4th years of the Doctoral studies. The PI will support the PhD candidate in preparing the application for this additional stipend. The amount of this additional stipend is 4242 PLN/month during until the end of 2nd year of PhD studies, increasing to 5340.90 PLN/month in years 3 and 4.

Required documents:

- Cover letter highlighting previous research experience and explaining the suitability of the candidate for the advertised position.
- CV
- Scan of the Masters' degree certificate (if already available)
- Contact details of two referees.
- Signed consent for the processing of personal data by the University of Warsaw.

Please email all the documents **no later than 5/03/2025** to **m.arhangelskis@uw.edu.pl** with a subject "**PhD application CSP**". Applications submitted after the deadline will not be considered. Selected candidates will be informed about the date of the interview by e-mail no later than **14/03/2025**. Interviews will be conducted remotely. Following the interview, the selected candidate will be appointed to the Doctoral School of Exact and Natural Sciences of the University of Warsaw.

……..……..
given and family name

Information on personal data processing

Controller
Controller of your personal data processed in connection with the recruitment process is the University of Warsaw, ul. Krakowskie Przedmieście 26/28, 00-927 Warszawa, as the Employer.

Contact with the controller:

- by traditional mail at: University of Warsaw, ul. Krakowskie Przedmieście 26/28, 00-927 Warszawa (name the organizational unit to which your letter is addressed);
- by phone: 22 55 20 355.

Data Protection Officer (DPO)
Controller has designated Data Protection Officer whom you may contact via email at iod@adm.uw.edu.pl. You may contact the DPO in all matters relating to your personal data processing by the University of Warsaw and the exercise of rights in relation to the processing of personal data.

The DPO, however, does not proceed other matters, like handling recruitment procedures, collecting recruitment documents, providing information on current recruitment process.

Purpose and legal grounds of data processing
Personal data of candidates for employment shall be processed for recruitment purposes only.

Your personal data shall be processed in the scope as indicated by employment law[1] (given name (names) and family name, date of birth, contact information as provided, education, professional qualifications, previous employment) for the purposes of this recruitment process[2], whereas other data[3] shall be processed based on your consent which may take the following wording:

I agree to the processing of personal data provided in .... (e.g. CV, cover letter, and other submitted documents) by the University of Warsaw for realising my recruitment process.

[1] Art. 22[1] of the law of June 26, 1974 Labour Code (i.e. Journal of Laws 2019 item 1040 with subsequent changes);
[2] Art. 6 section 1 letter b of the Regulation of the European Parliament and the Council (EU) 2016/679 of April 27, 2016 on protection of individual persons with regard to the personal data processing and on the free flow of such data, and also repealing Directive 95/46/EC (general regulation on data protection) (Official Journal EU L 119 of 04.05.2016, page 1, with subsequent changes) (hereinafter as the GDPR);
[3] Art. 6 section 1 letter a of the GDPR;

If your documents include data as mentioned in Art. 9 section 1 of the GDPR (special categories of personal data), processing shall be possible upon your consent to processing such data[4] which may take the following wording:

I agree to the processing of special categories of personal data, as mentioned in Art. 9 section 1 of the GDPR, provided in ..... (e.g. CV, cover letter, and other submitted documents) by the University of Warsaw for realising my recruitment process.

The University of Warsaw shall be also processing your personal data in future recruitment processes upon your consent[5] which may take the following wording:

I consent to processing of my personal data for the purposes of any future recruitment processes at the University of Warsaw for the period of the next nine months.

You may revoke all such consents at any time by, for example, sending an email at ..... (email address due for the recruitment process).

Be advised that the revocation of your consent does not affect legal compliance of processing which had been completed upon consent before its revocation.[6]

Data retention period

Your personal data collected in this recruitment process shall be stored over the period of three months from the date the recruitment process is completed.

In case you agree to process your data in future recruitments, your data shall be used over the period of nine months.

Data recipients

Officers authorized by the Controller shall have access to your personal data, the processing of which is in the scope of their duties.

Recipients of personal data may be other subjects obligated by the Controller to provide specific services involving data processing, like
.....
(name all recipients of data)

Data transfer outside the European Economic Area (EEA)

Your personal data shall be disclosed to subjects authorized by law. Signing-in is through Google Forms. Your personal data may be also processed by our provider of G-Suit for education by Google Company in their data processing centres.[7] Your data

[4] Art. 9 section 2 letter a GDPR;
[5] Art. 6 section 1 letter a GDPR;
[6] Art. 7 section 3 GDPR;
[7] https://www.google.com/about/datacenters/inside/locations/index.html

shall be protected under the standards of the Privacy Shield, accepted by the European Commission.[8] This shall guarantee an adequate level of data security.

Rights of the data subject
Under the GDPR data subjects have the following rights:

- *to access data and to receive copies of the actual data;*
- *to* correct (rectify) your personal data;
- to restrict processing of personal data;
- to erase personal data, subject to provisions of Art. 17 section 3 of the GDPR;
- to file a claim with the President of the Personal Data Protection Office, if you believe data processing violates law.

Information on the requirement to provide data
Providing your personal data in the scope resulting from law is necessary to participate in the recruitment process. Providing other personal data is voluntary.

.....
….....
place and date
applicant's signature

[8] https://www.privacyshield.gov