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Warsaw, 11 June 2025

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An announcement for postdoc position

Position of postdoc in the project entitled "Computational design of next generation rocket fuels based on hypergolic metal-organic frameworks" financed by National Science Centre is open for application.
Project leader: dr hab. Mihails Arhangeliskis.

The post-doc (adiunkt w grupie pracowników badawczych) will run research in exact and natural sciences, in the discipline of chemical sciences. Available positions: 1

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. We have recently reported the first computational design of hypergolic MOFs using crystal structure prediction (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.

Yet, we are still missing the key element in our computational design protocol, since there is no general theory which would allow us to predict the hypergolicity of a given MOFs, i. e. a time between the contact with an oxidizer and the appearance of the flame. Since this hypergolic ignition delay (ID) is a key performance characteristic for viable solid fuels, we need to develop a reliable approach for predicting ID for the MOF structures generated by CSP.

The successful candidate will utilize CSP calculations in combination with machine-learning (ML) models for predicting the structures and properties of new types of hypergolic MOFs. For the CSP part of the project the post-doc candidate will collaborate with a PhD student involved in the project, while development of ML models for the prediction of energetic properties and hypergolic ignition delays will be the sole responsibility of the post-doc candidate.

Relevant publications:

- (1) Titi, H. M.; Marrett, J. M.; Dayaker, G.; Arhangeliskis, M.; Mottillo, C.; Morris, A. J.; Rachiero, G. P.; Frišćić, 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 (4), eaav9044. <https://doi.org/10.1126/sciadv.aav9044>
- (2) Titi, H. M.; Arhangeliskis, M.; Katsenis, A. D.; Mottillo, C.; Ayoub, G.; Do, J.-L.; Fidelli, A. M.; Rogers, R. D.; Frišćić, T. Metal–Organic Frameworks as Fuels for Advanced Applications: Evaluating and Modifying the Combustion Energy of Popular MOFs. *Chem. Mater.* **2019**, 31 (13), 4882–4888. <https://doi.org/10.1021/acs.chemmater.9b01488>
- (3) Darby, J. P.; Arhangeliskis, M.; Katsenis, A. D.; Marrett, J. M.; Frišćić, T.; Morris, A. J. *Ab Initio* Prediction of Metal-Organic Framework Structures. *Chem. Mater.* **2020**, 32 (13), 5835–5844. <https://doi.org/10.1021/acs.chemmater.0c01737>
- (4) Xu, Y.; Marrett, J. M.; Titi, H. M.; Darby, J. P.; Morris, A. J.; Frišćić, T.; Arhangeliskis, M. Experimentally Validated *Ab Initio* Crystal Structure Prediction of Novel Metal–Organic Framework Materials. *J. Am. Chem. Soc.* **2023**, 145 (6), 3515–3525. <https://doi.org/10.1021/jacs.2c12095>

We are looking for motivated candidates:

- with a PhD degree in chemistry or related sciences (required in the first day of work at the latest).
- Experience with materials simulations, particularly periodic DFT calculations.
- Experience in machine learning for structure and property prediction of materials.
- Strong command in written and spoken English.

The candidate must meet the requirements of art. 113 of the Act - Law on Higher Education and Science dated July 20, 2018 (Polish Journal of Laws of 2024, no. 1571).

Main duties:

- Build ML models for the prediction of hypergolic properties of metal-organic frameworks.
- Help the project leader in supervising the doctoral student, employed in the project.
- Maintain scientific documentation and prepare research publication.
- Present research results at scientific conferences.

We offer:

a temporary contract of employment with the University of Warsaw (full time position), planned period of employment from 1.10.2025 till 30.09.2026 (with possibility of extension for further two years). Salary will be paid from the NCN grant at an annual rate of 140 000 PLN pre-tax.

Required documents:

- Curriculum Vitae (CV),
- Cover letter, highlighting prior experience and suitability for the advertised position,
- Two reference contacts,
- Signed form concerning the information on the processing of personal data,
- Declaration of reading and acceptance of the rules for conducting competitions at the University of Warsaw.

Please submit the documents **no later than 18 July 2025** by email to m.arhangelskis@uw.edu.pl. In the subject please write "Postdoc application".

Selected candidates will be invited for an online interview shortly after the application deadline. Final offer will be made based on the results of the interview. Candidates will be informed about the results of the competition by e-mail no later than 20 September 2025

The competition is the first stage of the employment procedure as an academic teacher, and its positive outcome is the basis for further proceedings.

The University of Warsaw has a procedure for whistleblowers to report violations of the law and take follow-up action - Internal Reporting Procedure, attached to Order No. 94 of the Rector of the UW dated September 17, 2024 on the Law on Procedure for Whistleblowers to Report Violations of the Law and Take Follow-up Action at the University of Warsaw, published and available in the UW [Monitor of 2024, item 266](#).