UNIWERSYTET WARSZAWSKI
Wydział Chemii

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WCH.1210-……../201**9** **Warszawa (Poland) 25/07/2019**

Work offer for a PhD student position

Position of a **PhD student** in the project entitled "***Ab initio* prediction of structures and properties of metal-organic frameworks for sensor applications**" financed by **National Science Centre (NCN)** is open for applications. The PhD candidate will be supervised by Dr. Mihails Arhangelskis, becoming a member of a newly established team for computational materials design within the Crystallochemistry laboratory (group leader Prof. Dr. hab. Krzysztof Woźniak).

Project leader: **Dr. Mihails Arhangelskis**

Grant Decision: **NR DEC-2018/31/D/ST5/03619**

Available positions: 1.

Abstract of the project: „ *Ab initio* prediction of structures and properties of metal-organic frameworks for sensor applications".

The principle aim of the project is the development of reliable methods for the computational design of metal organic frameworks (MOFs), which are highly versatile microporous materials, with applications in gas storage and separation, catalysis, energy storage and sensor devices. The broad range of applications stems from the modular nature of MOFs which are constructed from metal nodes (individual atoms or clusters) interconnected by organic linkers. The large choice of available nodes and linkers leads to essentially infinite number of topologies and, ultimately, properties. The question is, how do we find the right combinations of metals and linkers to build MOFs for specific applications?

Currently, the most common answer is experimental screening, which is not an optimal solution due to high costs and excess chemical waste. Our aim is to optimise the design of new MOFs by utilising computational methods. In a collaboration with Dr. Andrew Morris (University of Birmingham, UK) we have developed a method[1,2] for *ab initio* crystal structure prediction of MOFs, demonstrating that crystal structure of MOFs can be predicted solely based on the knowledge of chemical structure of nodes and linkers.

The PhD candidate will support the development of our methodology of MOF structure prediction, with the aim of improving accuracy and efficiency of our calculations and targeting the computational design of MOFs for sensor applications. At the same time, experimental synthesis of MOFs will be conducted to verify the

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correctness of our theoretical predictions, giving the candidate a solid background in both computational and experimental aspects of MOF development. The work will be conducted in collaboration with Dr. Andrew Morris (University of Birmingham, UK) and Prof. Tomislav Friščić (McGill University, Canada)

The candidate will be exposed to state-of-the-art methods of computational materials modelling and structure prediction as well as a diverse range of experimental synthetic and characterisation techniques. In particular, mechanochemical methods will be used to synthesise MOFs[3,4] alongside solution crystallisation. The candidate will also gain experience in high resolution X-ray diffraction measurements and quantum crystallography, dwelling on the state-of-the art instrumental facilities and expertise of the Crystallochemistry laboratory.

To enquire about the project please email marhangelskis@chem.uw.edu.pl. For further information about Dr. Arhangelskis and his research interests please visit: www.arhangelskis.org

References

(1) Darby, J. P.; Arhangelskis, M.; Katsenis, A. D.; Marrett, J. M.; Friščić, T.; Morris, A. J. Ab Initio Prediction of Metal-Organic Framework Structures. *ChemRxiv* **2019**. https://doi.org/10.26434/chemrxiv.8204159.v2

(2) 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.

(3) Akimbekov, Z.; Katsenis, A. D.; Nagabhushana, G. P.; Ayoub, G.; Arhangelskis, M.; Morris, A. J.; Friščić, T.; Navrotsky, A. Experimental and Theoretical Evaluation of the Stability of True MOF Polymorphs Explains Their Mechanochemical Interconversions. *J. Am. Chem. Soc.* **2017**, *139*, 7952–7957.

(4) Arhangelskis, M.; Katsenis, A. D.; Novendra, N.; Akimbekov, Z.; Gandrath, D.; Marrett, J. M.; Ayoub, G.; Morris, A. J.; Farha, O. K.; Friščić, T.; et al. Theoretical Prediction and Experimental Evaluation of Topological Landscape and Thermodynamic Stability of a Fluorinated Zeolitic Imidazolate Framework. *Chem. Mater.* **2019**, *31*, 3777–3783.

We are looking for a motivated PhD candidate who will perform crystal structure prediction calculations of metal-organic frameworks (MOFs) using a recently developed algorithm, as well as perform synthesis and characterisation of MOF materials for experimental validation of theoretical predictions.

We are looking for a person with:

- MSc degree in chemistry, materials science or related fields
- Experience with quantum chemical calculations

- Experience with crystallisation techniques
- Ability to measure and process X-ray diffraction data
- Good command of spoken and written English

Skills that would be advantageous, but are not required:

- Experience with periodic DFT calculations
- Knowledge of programming languages, particularly Python
- Experience with various solid-state characterisation techniques, e. g. solid-state NMR, UV/Vis and fluorescence measurements, thermal analysis.

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 contract with the University of Warsaw from **4/11/2019 to 30/11/2022.** The successful candidate will receive a non-taxed stipend of 4500 PLN/month for the whole duration of the project (36 months).

Required documents:

- Cover letter highlighting previous research experience and explaining the suitability of the candidate for the advertised position.
- Curriculum vitae including a list of publications (if available).
- Two reference letters should be sent to marhangelskis@chem.uw.edu.pl directly by the referees.
- Signed consent for the processing of personal data by the University of Warsaw (see below).

Please email all the documents **no later than 15/09/2019** to **marhangelskis@chem.uw.edu.pl** with a subject “PhD application”. 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 **10/10/2019**. If necessary, interviews may be conducted remotely.

INFORMATION ON THE PROCESSING OF PERSONAL DATA

INFORMATION CLAUSE

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3. Your personal data will be processed for the purpose of carrying out a recruitment process and selecting an employee and concluding a contract for employment at the University of Warsaw;
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5. Provision of data in the scope stipulated in the Labor Code is mandatory, and the remaining data are processed according to your consent for processing of personal data;
6. The data will not be shared with any external entities;
7. The data will be stored until you withdraw your consent for processing of personal data;
8. You have the right to access your personal data, to rectify, erase them, restrict their processing, object to processing, and to withdraw the consent at any time;
9. You have the right to lodge a complaint to the President of the Office for the Protection of Personal Data.

CONSENT CLAUSE

I hereby consent to have my personal data processed by the University of Warsaw with its registered office at Krakowskie Przedmieście 26/28, 00-927 Warszawa for the purpose of carrying out a recruitment process and selecting an employee and concluding a contract for employment at the University of Warsaw.

I have been informed of my rights and duties. I understand that provision of my personal data is voluntary.

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(place and date) (signature of the person applying for employment)