Offer of a PhD studentship

Position of a **PhD student** in the project "**Theoretical design and prediction of phosphorescent emissive materials based on halogen bonding interactions and experimental verification of their properties**" financed by **National Science Centre (NCN)** is open for applications. The successful 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 number: 2020/37/B/ST5/02638

Available positions: 1.

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. We combine state of the art periodic DFT calculations with crystal structure prediction (CSP) methods to achieve these tasks for a variety of organic and metal-organic materials.

The current project is aimed at developing accurate computational methods for the design of halogen-bonded molecular materials. Halogen bonding, as an attractive supramolecular interaction between an electrophilic region (σ-hole) of a halogen atom donor and a nucleophilic atom or functional group of the acceptor molecule is an emerging tool in the supramolecular synthesis of multicomponent crystals utilizing heavy elements. An exciting effect of the presence of heavy halogen atoms in the crystal structures of halogen-bonded cocrystals is their ability to induce phosphorescent emission in the chromophore molecules which would otherwise display fluorescence.

Our aim is to introduce computational design of functional materials utilizing XB interactions. This will not only dramatically improve the design efficiency, but also take our understanding of structure-property relationships controlling the behavior of halogen-bonded crystalline solids to a new level. The project will combine advanced computational modelling (periodic and molecular DFT calculations) with experimental crystallographic studies, solid-state mechanochemical synthesis and optical characterization.

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The successful candidate will work in a multidisciplinary team, and will gain state of the art training in experimental synthesis and characterization of halogen-bonded materials, collection and interpretation of X-ray diffraction data including high resolution experimental charge density analysis. In terms of theoretical calculations, the candidate will learn about periodic DFT modelling of crystalline materials for predicting their thermodynamic stability, calculating intermolecular interaction energies, as well as modelling optical and luminescent properties. The wide range of techniques covered in this project provides an excellent preparation for future career in crystal engineering and materials design, either in academia or in industry.

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

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) Arhangelskis, M.; Jochym, D. B.; Bernasconi, L.; Friščić, T.; Morris, A. J.; Jones, W. Time-Dependent Density-Functional Theory for Modeling Solid-State Fluorescence Emission of Organic Multicomponent Crystals. *J. Phys. Chem. A* **2018**, *122*, 7514–7521.
(2) Lisac, K.; Topić, F.; Arhangelskis, M.; Cepić, S.; Julien, P. A.; Nickels, C. W.; Morris, A. J.; Friščić, T.; Cinčić, D. Halogen-Bonded Cocrystallization with Phosphorus, Arsenic and Antimony Acceptors. *Nat. Commun.* **2019**, *10*, 61.
(3) Topić, F.; Lisac, K.; Arhangelskis, M.; Rissanen, K.; Cinčić, D.; Friščić, T. Cocrystal Trimorphism as a Consequence of the Orthogonality of Halogen- and Hydrogen-Bonds Synthons. *Chem. Commun.* **2019**, *55*, 14066–14069.
(4) Arhangelskis, M.; Topić, F.; Hindle, P.; Tran, R.; Morris, A. J.; Cinčić, D.; Friščić, T. Mechanochemical Reactions of Cocrystals: Comparing Theory with Experiment in the Making and Breaking of Halogen Bonds in the Solid State. *Chem. Commun.* **2020**, *56*, 8293–8296.

Necessary qualifications:
- MSc degree in chemistry, materials science or related fields
- Experience with crystallization techniques and (optionally) mechanochemistry
- Experience with quantum chemical calculations
- Good command of spoken and written English

Additional skills which would be advantageous:
- Ability to measure and process X-ray diffraction data
- Experience with periodic DFT calculations
- Experience with various solid-state characterization 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 36 month contract with the University of Warsaw, starting from October 2021. The successful candidate will receive a stipend of 5000 PLN/month (3716.16 PLN/month after social security deductions) for the whole duration of the project.

There is also a possibility to receive additional stipend from the University of Warsaw Doctoral School of Exact and Natural Sciences. For this the successful candidate will be encouraged to apply via the Doctoral school, where the application deadline will be 28/06/2020. The amount of this additional stipend is 2371.70 PLN/month during 1st and 2nd year of PhD studies, increasing to 3653.70 PLN/month in the subsequent years.

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 10/05/2021** to **m.arhangelskis@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 **25/05/2021**. Interviews will be conducted remotely.

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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:

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[1] Art. 22¹ 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;

> 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.

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

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[4] Art. 9 section 2 letter a GDPR;
[5] Art. 6 section 1 letter a GDPR;
[6] Art. 7 section 3 GDPR;

G-Suit for education by Google Company in their data processing centres.[7] Your data 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.

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

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[7] https://www.google.com/about/datacenters/inside/locations/index.html
[8] https://www.privacyshield.gov