

**Job offer:** scholarship position, PhD student type in Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw

**Requirements:**

We seek a motivated candidate with a MSc (or equivalent) degree in chemistry, physics or related field and a strong theoretical chemistry or physics background. The knowledge of English allowing to read scientific literature is required. The knowledge of a programming language and Linux is an additional asset.

**General information about the project:** The position is funded by a grant from the National Centre of Science (Poland; OPUS program, title: *Properties and reactivity of molecules and molecular complexes under partial spatial confinement*, decision No. DEC-2017/27/B/ST4/02699) coordinated by Dr. hab. Tatiana Korona.

The main objective of this project consists of a development of a new approach for calculating molecular properties of first and second order, which will be based on an existing approach of systematic molecular fragmentation (SMF) for electronic energies, and the application of ab initio electron-correlated methods for the calculation of these properties within the SMF. The main testing ground of the new method will be molecular complexes composed of a smaller molecule (guest) partially enclosed in a larger molecule (host). Such systems represent an intermediate case between usual intermolecular complexes and fully endohedral ones. It should be noted that such complexes are of great interest for chemists and biologists and a possibility of an accurate description of their properties is therefore of a great importance. To this end, the second major objective of this research will be an investigation of several real-life complexes, such as e.g. complexes with calixarenes acting as hosts, in order to provide a new insight into changes of properties of both host and guest resulting from their mutual interaction.

**Job duties:** The position will involve application and extensions of the systematic molecular fragmentation model to calculate molecular properties and studying the relationship between SMF and embedding theory. The student's tasks will involve: performing calculations with selected quantum chemistry packages, programming interfaces between the SMF and these packages, designing models capable to handle molecular properties based on the SMF approach, as well as designing performance tests and making applications of the novel methods.

**Employment conditions:**

- total scholarship per month: 4500 PLN
- employment period: max. 36 months
- financing of scientific conference attendance
- after successful recruitment, the candidate will have to obtain the status of PhD student at the Faculty of Chemistry of the University of Warsaw (see <http://www.chem.uw.edu.pl/kandydaci/studia-doktoranckie/>, in case of problems with translation please contact me (T. Korona) )

**Required documents:**

- CV
- a copy of diploma
- a transcript of record from undergraduate studies- motivation letter
- recommendation letter from diploma thesis advisor and his/her contact details
- personal data processing agreement clause (see below)

**How to apply information:**

Applications should be submitted by e-mail to Tatiana Korona ([tania@chem.uw.edu.pl](mailto:tania@chem.uw.edu.pl)) no later than 2nd of September 2018. Selected candidates will be invited for a job interview (Skype/phone form possible).

The results will be announced at 4th of September 2018.

**Contact details:** Dr hab. Tatiana Korona, Pracownia Chemii Kwantowej, Wydział Chemii Uniwersytetu Warszawskiego (p. 505), ul. Pasteura 1, 02-093 Warszawa. E-mail: [tania@chem.uw.edu.pl](mailto:tania@chem.uw.edu.pl), <http://tiger.chem.uw.edu.pl/index.php?i=tania>

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**INFORMATION CLAUSE**

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2. The Controller has designated the Data Protection Officer who supervises the processing of personal data, and who can be contacted via the following e-mail address: [iod@adm.uw.edu.pl](mailto:iod@adm.uw.edu.pl);
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;
4. The provided data will be processed pursuant to Article 22<sup>1</sup> § 1 of the Act of 26 June 1974 Labor Code (uniformed text: Dz.U. of 2018, item 917) and your consent for processing of personal data;
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 ul. 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.

.....  
(place and date)

.....  
(signature of the person applying for employment)