

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

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) no later than 31st of July 2018. Selected candidates will be invited for a job interview (Skype/phone form possible).

The results will be announced at 14th of August 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, <http://tiger.chem.uw.edu.pl/index.php?i=tania>

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(place and date)

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