

Keywords:

development of computer package; computational modeling

Scholarship Offer for MSc or PhD Student at Faculty of Chemistry, A. Mickiewicz University, in Project Opus 11

Adam Mickiewicz University in Poznań announces an open competition for the position of MSc (*Magistrant - stypendysta*) or PhD student (*Doktorant - stypendysta*) in Faculty of Chemistry. The selected candidate will realize the research tasks in the project OPUS 11: "*Rational design of molecular nanomagnets: synthesis, characterization, theoretical description and computational modeling of their properties*" (financed by the National Science Centre under the terms of the Agreement for this project). Major task is to provide **computational support** leading to better understanding and prediction of spectroscopic and magnetic properties of molecular nanomagnets (MNM) using semiempirical methods.

Scholarship Offer for MSc or PhD Student at Faculty of Chemistry, A. Mickiewicz University, in Project Opus 11

Institution: Faculty of Chemistry, Adam Mickiewicz University in Poznań

Position Name: MSc (*Magistrant - stypendysta*) or PhD student (*Doktorant - stypendysta*) in the project OPUS 11: "*Rational design of molecular nanomagnets: synthesis, characterization, theoretical description and computational modeling of their properties*".

Duration: till 28th of February 2022, not shorter than 6 months

Salary: MSc student 800 PLN/month (gross); PhD student 1620 PLN/month (gross).

Principal Investigator (and Supervisor): Prof. Czesław Rudowicz.

Requirements:

- Practical experience in programming using suitable computational languages, e.g. Fortran.
- Other qualifications required:
 - experience in programming using MathCad would be an advantage;
 - basic knowledge of fundamentals of crystallography, symmetry and group theory;
 - high level of analytical skills and inquiring mind.

Scope of work within project tasks:

- Further development of computer package for analysis of low symmetry aspects in the zero field splitting parameter (ZFSP) sets or crystal field parameter (CFP) sets for the 3d/4f ions in crystals and molecules.
- Carrying out calculations using the extended computer package, including
 - standardization of the orthorhombic, monoclinic, and triclinic ZFSP/CFP sets to ensure comparability of disparate sets taken from various sources;
 - comparative analysis of low symmetry aspects inherent in the triclinic or monoclinic ZFSP/CFP sets obtained by us or reported in literature for the constituent 3d/4f ions in selected molecular nanomagnets (MNM);
 - analysis of low symmetry aspects based on crystallographic data (cif files) using, e.g. SYMMOL computer package.

Additional information:

- Application containing: motivation letter, CV (including photo), publication list (if any), copy of diploma (if available, or information on current status of MSc or PhD thesis), contact details of 2 potential referees, should be sent as a single pdf-file or zip-file. Please include in your application one page with the following phrase: "*In accordance with Article 6(1)(a) of the General Data Protection Regulation of 27 April 2016 (Journal of Laws of the EU L 119/1 of 4 May 2016) I agree to the processing of personal data other than those indicated in Article 221 of the Labour Code (name(s) and surname; parents' names; date of*

birth; place of residence; address for correspondence; education; previous employment), included in my job offer for the purpose of current recruitment."

- Selected candidates may be invited for the interview – the date will be communicated to the candidates individually.

Send applications by email to: <czerud@amu.edu.pl> *with a copy to*
<kinga.roszak@amu.edu.pl>

The e-mail heading should be: "MSc/PhD student #4C–OPUS grant".

Application deadline: 20.04.2021 or until position is filled in.

For more information, contact: Prof. Czesław Rudowicz by email: <czerud@amu.edu.pl>.