

**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>.