

Project title: New extensions and applications of symmetry adapted perturbation theory

Position: PhD-scholarship

Number of positions: 1

City: Toruń

Website: <https://www.fizyka.umk.pl/en>

Requirements:

The project will involve implementing and testing new SAPT developments using Python, including new interaction-energy expressions, density-matrix-based approaches, molecular properties, numerical algorithms, and benchmarking against reference calculations.

A solid background in quantum chemistry and molecular interaction theory is essential. Good knowledge of Python and experience with electronic-structure calculations are also required.

The project is suitable for a student interested in intermolecular forces, electronic-structure theory, and scientific programming, and will involve close collaboration with researchers developing modern SAPT methodology.

Description of duties - Tasks:

- Development and implementation of SAPT/SART induction-energy expressions, including higher-order polarization effects beyond standard low-order SAPT.
- Implementation of self-consistent monomer response in the field of the interacting partner, providing induction energy summed to infinite order within the SART framework.
- Analysis of the connection between induction, polarization, and charge-transfer contributions, including the role of orbital/density relaxation and projection schemes.
- Numerical implementation and benchmarking in Psi4/Python, with comparison against conventional SAPT induction terms, supermolecular calculations, and reference interaction energies.

Competition type: Osonata Bis 9

Field of science: np. ST

Application deadline: 15.10.2026 23:59

Application form: e-mail

Employment conditions:

A scholarship in the amount of PLN 5 000 per month.

Planned period of employment: 5 months

Additional information:

The scholarship is awarded in accordance with the rules set out in the Regulations on the Award of Research Scholarships of the National Science Centre, adopted by Resolution No. 25/2019 of the Council of the National Science Centre dated 14 March 2019.

Required documents (send to : pzuch@fizyka.umk.pl/with annotation "Sonata Bis 9.1"):

- Cover letter
- CV
- Copies of obtained diplomas and certificates (if any)
- Copy or scan of candidate's publications (if any)
- Information about scientific awards, scholarships and other distinctions (if any)
- Description of current research activity (if applicable)
- Consent to the processing of personal data (EN):
https://view.officeapps.live.com/op/view.aspx?src=https%3A%2F%2Fwww.umk.pl%2Fen%2Fjobs%2Fdocs%2Fen_os4.docx&wdOrigin=BROWSELINK
PL: <https://www.fizyka.umk.pl/panel/wp-content/uploads/Zalacznik-bez-tytulu-00016.pdf>
- Certificate of student status/ PhD student

Applicants will be evaluated by a selection committee appointed by the Dean of the Faculty of Physics, Astronomy and Informatics. The committee will recommend the awarding (or rejection) of the scholarship no later than 16.10.2026 r.

Candidates will be notified of the outcome of the competition by e-mail.

In the event of resignation of the selected candidate, the right to indicate the next candidate from the ranking list is reserved.

All documents should contain the candidate's signature or its scan.

Language of application: Polish or English.