



# Institute of Physics of the Polish Academy of Sciences

## Scholarship for a PhD Student



**Job ID: #JOB 60/2022**

**Job Description:** PhD student – scholarship holder

**Job Title:** Ab initio investigations of Hund's Rule breaking organic molecules

### Job Summary:

#### Job Description:

The main scientific goal of the project bases on extensive ab initio computational explorations of novel, so-far unknown, organic compounds exhibiting the  $S_1/T_1$  inversion in order to understand fundamental mechanisms and to determine electronic and nuclear factors that govern this unexpected and rare phenomenon. This is almost completely unexplored field so far and the research will need the combination of chemical intuition in designing such systems with extensive computational work. Several wavefunction- and DFT- based methods of electronic structure theory such as MP2, ADC(2), CC2, CASSCF, UDFT, and TDDFT will be used for determination of molecular properties in the ground and in the lowest electronically excited states of theoretically designed polyatomic molecules.

The technical aim of the project is related to future OLED application of these systems, and will involve computational optimization of the  $S_1 \rightarrow S_0$  fluorescence intensity and wavelength of theoretically designed molecules with the restriction of a negative singlet-triplet energy gap.

#### Requirements:

- Basic knowledge of wavefunction- and DFT- based methods of electronic structure theory such as MP2, CC2, CASSCF, and TDDFT.
- Some experience in running quantumchemical program packages like Gaussian, Turbomole or Molpro.
- Proficiency in English.
- Master's degree in physics or chemistry (or an equivalent that qualifies one for PhD studies in physics in the country of issue).
- To be employed, the candidate must be accepted into the PhD school in which the Institute of Physics participates. Applications for the position are through recruitment to the School, online at [warsaw4phd.eu](http://warsaw4phd.eu).

**Main research field:** Physics

**Sub Research Field:** Theoretical Chemistry

**Career Stage:** Early stage researcher or 0-4 yrs (Post-graduate)

**Research Profile ([details](#)):** First Stage Researcher (R1)

**Type of Contract:** Fixed term 24 months (with possibility of extension up to 48 months)

**Status:** Full-time

**Salary:** grant funding of **5000** PLN per month, before subtracting obligatory employer and employee social security contributions (~15%). (After 2 years possibility of prolongation under the standard Polish PhD scholarship, about 3240 PLN/month net in years 3-4)

## Contact

More information can be obtained from

Prof. Andrzej Sobolewski (e-mail: [sobola@ifpan.edu.pl](mailto:sobola@ifpan.edu.pl))

<http://www.ifpan.edu.pl/ON-2/on21.html>

Please make contact.

## Application details

**Application deadline: 04.01.2023** Later applications will not be considered.

**Required materials:**

- Scientific CV
- Cover letter
- Scan of MsC diploma or equivalent (or an explanation of when one is expected)
- Academic record (for finalized semesters)
- Recommended: A recommendation letter by an academic, or their contact email.

All materials should be submitted in electronic form by application to the PhD school [warsaw4phd.eu](http://warsaw4phd.eu), choosing the project: "*Ab initio investigations of Hund's Rule breaking organic molecules*". The application system will be active from 21 December 2022. Results regarding the position will be made available by 4 February 2023.