UNIVERSITY OF SILESIA
IN KATOWICE

PHD STUDENT IN THE DOCTORAL SCHOOL – CALL FOR APPLICATIONS

Position: PhD student in **Materials Science and Engineering** discipline

Unit of the project realization: **Faculty of Science and Technology** – University of Silesia in Katowice

Unit realizing the PhD student education: Doctoral School at the University of Silesia in Katowice

Short description of the job

The main goal of the project is to determine the relationship between the molecular structure and the resulting macroscopic properties of the liquid crystal material

The tasks of the doctoral student will include an experimental work - characterization of materials using Polarizing Microscopy, infrared (FTIR) and Raman spectroscopy, structural studies using X-ray diffraction (SAXS, WAXS) - Performing calculations using the quantum mechanics modeling method (DFT), writing scientific papers, active participation in international conferences. As part of the project, an internship at Toyohashi University of Technology in Japan is planned.

Research will be carried out in the frame of the project „ **The role of intermolecular interactions, molecular bend angle and biaxiality in stabilizing the structure of the twist-bend phase liquid crystal materials.**", financed from **Preludium BIS 2, No. 2020/39/O/ST5/03460** under management of **dr hab. Katarzynay Merkel, prof. UŚ.**

Duration of the scholarship: 48 months

Scholarship amount: 4,266.58 PLN (gross), after evaluation 5,119.89 PLN (gross)

Deadline for submitting documents: July 14, 2021, 23:59

The deadline for adjudication of the competition: July 19, 2021, 12:00

Planned date of commencement of works in the project: October 1, 2021

Project description:

The twist-bend nematic phase (N_{TB}) is a rare example of a chiral structure that occurs as a result of the spontaneous symmetry breaking of non-chiral banana-shaped moleules in a system without long-range positional ordering. In the nematic twist-bend spatially modulated phase, the director forms a conical helix with a pitch of several to tens of nanometers, in which the director, i.e. the mean direction of the long axes of the molecules, is inclined with respect to the helix axis at an angle (usually <35°). It can be said that this phase is a kind of the bridge between the classic nematic phase and the cholesteric phase. Despite extensive research, many properties of the N_{TB} phase and their relationship to the molecular structure have still not been established and understood. Particularly interesting is the role of the molecular bending molecules in the N_{TB} phase formation and stability, and the key molecular feature that determines it is the nature of the connecting group between the rigid core and the linker. Recent reports show that the angle of bending of molecules has a clear

influence on the molecular biaxiality, which means that the molecules in the system are ordered in relation to two mutually perpendicular directions. The biaxiality may be directly related to the periodicity of the helical structure. By determining molecular biaxiality using infrared spectroscopy, we can predict the twist-bend helix jump. The latter parameter is of great importance for the application of materials with the N_{TB} phase, because the helicoid period is in the nanometer range, and therefore the expected electro-optical response time is very short and amounts to about 1μs, so many times shorter compared to the response time for conventional nematic materials. The project presents an innovative approach to a comprehensive description of the macroscopic properties of a material based on their molecular properties. The main goal of the project will be to determine the relationship between the molecular structure and the resulting macroscopic properties of the material.

The role of a PhD student:

• The experimental work will include: characterization of materials using Polarizing Microscopy, optical birefringence measurements, measurements of infrared (FTIR) and Raman spectra, structural studies of local order using X-ray diffraction (SAXS, WAXS)
• Performing calculations using the quantum mechanics modeling method (DFT) to study the electronic structures of molecules. Determination of the theoretical infrared spectra and energy of intermolecular interactions.
• Writing scientific papers, active participation in international conferences.
• Preparation and defense of the doctoral dissertation on the dates compliant with the documentation of the Preludium BIS 2 competition.

Requirements:

1. Title of Master's, Master engineer or equivalent – during admission the candidate may provide a certificate of obtaining a master's degree.
2. Thesis subject related to liquid crystal materials in the field of materials science, chemistry or physics.
3. Knowledge of experimental techniques: such as: FTIR or Raman spectroscopy, polarizing optical microscopy.
4. Knowledge of computational methods of quantum chemistry.
5. Knowledge of design tools and fluency in using the Origin program are welcome
6. Ability to write scientific texts in English
7. English language certificate at least at B2 level, allowing you to read the scientific literature freely.
8. Resourcefulness, motivation and great commitment to research work.

Required application documents:

1. Cover letter with a description of scientific interests.
2. CV.
3. List of publications to date with a description of the candidate's contribution or other scientific achievements (participation in conferences, awards, scholarships and other awards).

4. A copy of the diploma or a certificate confirming obtaining the degree.
5. Two reference contacts.

Additional information:

Documents should be delivered till July **14th 2021** to an e-mail: **katarzyna.merkel@us.edu.pl**
In case of any questions, before the formal application please contact to the grant leader for the e-mail address given above.
Documents will be rated by the commission, led by the project leader. Admission will be carried out according to the NCN regulations. Admission can be carried out both in Polish and in English. Meeting will be organized on **15.07.2021** in the Doctoral School office / on-line. Final decision will be sent to candidates via e-mail till **19.07.2021.**