



Přírodovědecká
fakulta
Faculty
of Science

Jihočeská univerzita
v Českých Budějovicích
University of South Bohemia
in České Budějovice

Postdoctoral position: Computer modelling of nonlinear optics signals at interfaces

Terms and location:

Applications are invited for a postdoctoral position at [Department of Physics](#) at [Faculty of Science](#) of [University of South Bohemia](#) in [Ceske Budejovice](#) (Czech Republic).

The position for a postdoc working on a project “**Computer modeling of nonlinear optics signals at interfaces**” is open immediately. The duration of this project funded by the Czech Science Foundation (GACR) is 01/2022-12/2024.

The position is offered for an initial period of one year with a possible (and anticipated) extension till 12/2024.

Information about the Principle Investigator of the project, Milan Predota, can be found here: <https://web.prf.jcu.cz/en/ufy/structure/people/predota.html>

Abstract of the project: Originating exclusively in non-centrosymmetric environments, Sum Frequency Generation (SFG) and Second Harmonic Scattering (SHS) generation have become powerful and extremely sensitive techniques for studying processes at surfaces and interfaces. Improved methods, models, and necessary input parameterizations from ab initio calculations will allow prediction and interpretation of the SFG spectra of aqueous solutions and to develop modelling of SHS signals. We advance our cooperation with experimental and ab initio calculations experts from the study of planar inorganic interfaces (crystalline and amorphous metal oxides) towards the study of dispersed nanoparticles and soft organic interfaces (organic self-assembled monolayers, lipid membranes). Our aim is to allow the prediction of nonlinear spectra of much larger systems and on a much longer time scale than ab initio methods allow, towards biologically relevant systems. Linking experimental results with a molecular description of the origin of spectroscopic signals will lead to a better understanding of the interfacial phenomena.

The successful candidate will predict and determine nonlinear optics spectra from molecular dynamics simulations at the aqueous interfaces of solids, colloidal particles, and organic surfaces, and compare them with experimental spectra; improve methods allowing determination of non-linear optics signals from computer simulations. He/she will combine the theory of the SFG and SHS signals with simulation data obtained for the interfaces to predict the resulting spectra.

Requirements:

- A PhD in physics, chemistry, materials science, or related field, obtained not before Jan 1 2014 (extensions apply due to maternity and parental leave, and sick leave in the case of a long-term illness)
- A strong background in computational physics or chemistry
- Proficiency in classical molecular dynamics (best in Gromacs, LAMMPS) and/or ab initio calculations (best in CP2K, VASP)

- Proficiency in programming of scientific codes (best in FORTRAN, C)
- Ability to learn the theory of non-linear optics
- Excellent communication skills and a career level-appropriate publication track record
- The ability to work independently and collaboratively in a research team

Applications:

The project will be supervised by Assoc. Prof. Milan Predota, predota@prf.jcu.cz.

The applications should be submitted to Ms. Aneta Hanusova, jobs@prf.jcu.cz.

The applications should include:

- (i) CV in PDF format,
- (ii) a motivation letter briefly describing your research achievements,
- (iii) complete list of publications, and
- (iv) contacts to one or two senior scientists who could possibly provide recommendation letters upon our request.

For further information about the position, please feel free to directly contact Milan Predota. Use "Postdoc-NLO" as subject in your e-mail communication.

Review of applications begins immediately. Applications are accepted until the position is filled.

June 8, 2022