



## Postdoctoral Position in development of QM/MM simulations of organic molecules on ionic substrates

The Institute of Physics of the Czech Academy of Sciences is looking for a new colleague to work on integration of DFT/DFTB methods with classical force fields into QM/MM package as a part of project “**Computer Aided Design of Templated Assembling, Replication and Synthesis on Ionic Substrates**”. The project aims to computationally develop an universal molecular architecture for assembling molecular components into larger functional systems (e.g. computer circuits) on ionic substrates.

### Job description

- integration of DFT/DFTB methods with classical force-fields into QM/MM package
- testing of various approximations and fitting empirical parameters
- development of high-throughput screening workflow to find optimal molecular designs
- data analysis of computational results
- co-supervising 2 PhD students running most of QM/MM calculations

### Your profile

- PhD in computational solid state physics or chemistry
- Programming, e.g.: C/C++, Python (numpy), Fortran, GPU (OpenCL/CUDA)
- experience with development of molecular simulations (either quantum or classical)
- previous experience with QM/MM considered a strong advantage!
- good spoken and written English
- keen to learn new simulation methods, ability to solve problems independently

### We offer

- opportunity to achieve a major breakthrough in nanofabrication
- contract may be prolonged up to 4 years (till 2026)
- work in an international and creative environment
- active participation at international workshops and conferences
- training and development opportunities (soft skills, language courses)
- flexible working hours with home office possibility
- 5 weeks of vacation + 6 sick days a year
- plenty of opportunities for cultural and other activities in the Prague region
- more information is available at: [Why FZU?](#)

### How to apply

Contact [Prokop Hapala](#) ([hapala@fzu.cz](mailto:hapala@fzu.cz)) to discuss details of the research project. Your formal application send to [kariera@fzu.cz](mailto:kariera@fzu.cz) by **30.1.2022** and include

- cover letter explaining your motivation and interests
- CV with your research experience and a list of publications
- proof of programming skills (e.g. link to git repository or similar)
- names and e-mail addresses of two established scientists who could be asked for reference

The starting date is flexible during Summer 2022. For general employment information contact to Lucie Beránková ([berankova@fzu.cz](mailto:berankova@fzu.cz)).

## About the Institute

The Institute of Physics of the Czech Academy of Sciences (FZU) is a public research institution specializing in fundamental and applied research in physics, especially elementary particle physics, condensed matter physics, solid state physics, optics, plasma physics and laser physics. The FZU is the largest institute of the Czech Academy of Sciences with more than 1300 employees, including a considerable number of international workers. As a public research institution, the FZU contributes to increasing the level of knowledge, the quality of education, and the use of research findings in practice.

On April 2019, the FZU has become a holder of the certificate *HR Excellence in Research Award*, which is awarded by the European Commission. The FZU has thus ranked among the group of prestigious European institutions having the right to use this certificate.