



PhD Student Position in Computational Catalysis (Chemistry/Physics)

Department of Catalysis and Chemical Reaction Engineering at the National Institute of Chemistry, Ljubljana, Slovenia is offering a **full-time PhD Student Position** (m/f) for a period of **3 years**, starting in May 2019 or later upon the agreement with the selected candidate (at the latest in October 2019).

Content of work:

We are offering a PhD position for candidates with master's degree in chemistry, physics, chemical engineering or related areas. The content of the work includes computational modelling of chemical reactions at various time and length scales (atomistic scale, meso-scale) in heterogeneous catalysis. The candidate will be primarily involved in theoretical studies of catalytic systems on the atomistic scale. The candidate will work on a H2020 project (BiZeolCat) and investigate the catalytic dehydrogenation of butane and propane. The research work will consist of *in silico* studying catalytic surfaces, mapping out reaction pathways, calculating reaction rates and simulating the whole catalytic process.

The candidate will have the opportunity to work on a state-of-the-art high-performance computing cluster. The candidate will collaborate closely with experimentalists at the department.

Experience or interest in atomistic modelling of chemical reactions, including kinetics and thermodynamics, is beneficial. A solid background in statistical physics and physical chemistry is an advantage. The candidate should be fond of working with computers. Knowledge of open-source software (Linux) and programming (Python, scripting) is an asset.

The candidate should be reliable, motivated, independent and resourceful. Good command of spoken and written English is required and can be demonstrated through language skill certificates or application-enclosed publications (preferably first-authored).

Please send your application by e-mail (matej.hus@ki.si) and enclose 1) a **CV** (with relevant scientific and research background), 2) a **cover letter** and 3) **university certificates** (if the candidate does not have a master's degree yet, a statement that one will be obtained before 30 September is required).

More information about the department: <https://www.ki.si/en/odseki/d13-odsek-za-katalizo-in-reakcijsko-inzenirstvo/>.

The closing date for this application is 31 March 2019.

Number of positions available: 1

Research Fields

Computational Chemistry, Chemical Physics, Chemical Reaction Engineering

Career Stage

Candidate with a master's degree.

Research Profile

Recognised Researcher (R1)