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Topics for the Janko Jamnik Doctoral Scholarship for Promising Early-Stage Researchers in Chemistry and Related Sciences for 2019

Topic Title	Short Content	Mentor	Department
Conversion of Carbon Dioxide Into Monomers	Nowadays, the main building blocks of plastic or rubber (ethene, propene, butadiene...) are extracted from petroleum. The content of the doctoral thesis would include the conversion of CO_2 into monomers, through the development of catalytic converters, chemical reaction engineering, and modelling.	Blaž Likozar	D13/D09
Photo-Catalytic Preparation of Bio-Based Green Compounds	Today, most substances are produced from fossil raw materials using wasteful processes, while photocatalysis is based on the use of solar energy that would be used to convert bio-based compounds from biomass.	Blaž Likozar	D13/D09
Procedures For Electrocatalytic Conversion of CO_2	In addition to biomass, CO_2 is the only permanent source of carbon raw materials, but today it is being converted to, for example, methanol, urea..., for which we need hydrogen, obtained by electrolysis - direct electro-catalytic conversion provides for significant improvement.	Blaž Likozar	D13/D10
Synthesis and Advanced Study of the Activity, Stability and Selectivity of Electrocatalysts for the Conversion of Atmospheric Nitrogen	The global energy crisis and consequent climate change will result in reduced consumption of fossil fuels and an increased use of alternative energy sources such as solar energy. A major challenge for the future will be the conversion or storage of excess solar energy. In addition to the electrolysis of water and electroreduction of CO_2, an electrochemical conversion of atmospheric nitrogen, which represents 78% of the air, into compounds with added value, is also offered here, thereby potentially replacing the Haber-Bosch process.	Nejc Hodnik	D13/D10
Organic Electrosynthesis	The research topic will deal with organic electrosynthesis. Using electrocatalysts, we will try to selectively synthesise organic compounds. Our goal is to offer an alternative to conventional, expensive and environmentally dangerous redox systems, which are currently used in classical organic synthesis.	Primož Jovanovič	D13/D10/D04

Three-Dimensional Macroporous Frames Based on Synthetic Polypeptides, Prepared by Emulsion Templating	The student will prepare synthetic polypeptides with different functionalities by polymerisation, by opening the ring. These will then be crosslinked in emulsions with a high proportion of the internal phase, thereby obtaining degradable macroporous frames, which will be further tested for use in tissue engineering.	David Pahovnik	D07/D11
Multiscale Simulations of Battery Systems	Theoretical modelling of electrode surfaces in electrochemical processes in next generation batteries: from atomic scale to kinetics on meso scale.	Drejc Kopač and Anja Kopač Lautar	D13 and D10
Modelling the Oxidation of Alkenes from Quantum Mechanics to the Industrial Criterion	The most important catalytic reaction of oxidation on an industrial scale is epoxidation. The reaction will be described using the methods of quantum physics, kinetic simulations and calculation dynamics of fluids, and then carried out experimentally.	Matej Huš	D13/D09
The Source of Entropy	In environmentally important reactions in the atmosphere, entropy plays a decisive role. Thermodynamics of reactions in atmospheric aerosols will be studied theoretically (quantum molecular dynamics, statistical thermodynamics) and experimentally (photolysis with laser beam).	Matej Huš	D13/D04/D01
Designing New Materials for Air Purification	PM particles are harmful to our health, affect the weather, and cause climate change. We will carefully study the interactions of PM particles from the atmosphere with different surfaces, and design new, affordable materials with distinctive air purifying properties in an energy efficient manner.	Ana Kroflič	D04/D10
Brown Carbon in the Atmosphere	Brown carbon - the absorbent part of organic aerosols - affects the absorption properties of the atmosphere and thus visibility, the ecosystem and, most importantly, climate change (greenhouse effect). We are interested in its identity, sources and secondary formation and ageing in the atmosphere.	Ana Kroflič	D04/D13

Dynamic Model of Human DNA Topoisomerase IIa and Development of New Catalytic Inhibitors As Anti-Cancer Agents	We will use methods of molecular simulations in combination with biochemical experiments, and study the mechanistic operation of the molecular engine of the human DNA topoisomerase IIa. Furthermore, we will plan and characterise new catalytic topo IIa inhibitors that would bind to the ATP binding site at the ATP domain and would be suitable for further preclinical development. Such an approach represents a new alternative to the topo IIa inhibition paradigm, which can lead to safer anti-cancer therapies.	D01/D11