KEMIJSKI INŠTITUT

Vabilo na Forum40 / Invitation to the Forum40

dr. Matej Huš

D13, Department of Catalysis and Chemical Reaction Engineering

Četrtek / Thursday, 4.6. 2020 ob / at 10:00 / on WEBEX

Meeting link: https://ki-si.webex.com/ki-si/j.php?MTID=m86cdf6c22a56477305cefba0eec7aff4

Meeting number (access code): 113 928 2678
Meeting password: kemijski

From atoms to reactors: multiscale modelling in catalysis

Recent advances in the available computing power have enabled us to describe chemical transformations on all levels. We can couple quantum chemical calculations at the electronic level with atomistic simulations, meso-scale simulations and a continuum description of whole reactors. This gives us unprecedented capabilities. We can discover and describe reactions mechanism and the corresponding kinetics. We can therefore advance past describing and start predicting optimum catalysts and reactor designs wholly computationally.

Vljudno vabljeni / Kindly invited