



Vabilo na Preglov kolokvij / Invitation to the Pregl colloquium

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Velika predavalnica Kemijskega inštituta /
Great Lecture Hall, National Institute of Chemistry;
Hajdrihova 19, Ljubljana, Slovenia

Structure-dependent microkinetic analysis of heterogeneous catalytic processes: methodology and applications

There is no doubt that the rational interpretation of the structure-activity relation in catalysis is a crucial task in the quest of engineering the chemical transformation at the molecular. In this respect, multiscale analysis based on structure-dependent microkinetic modelling is acknowledged to be the essential key-tool to achieve a detailed mechanistic understanding of the catalyst functionality. However, the effect of the structure of the catalyst on reactivity and selectivity is at present neglected in state-of-the-art microkinetic modelling.

In this talk, I will present the development of a methodology for the analysis of the structure-activity relation in heterogeneous catalysis by hierarchically combining methods at different levels of accuracy in a dual feed-back loop between theory and experiments. This includes the development of both novel experimental tools and first-principles analysis. Selected examples in the context of CH₄ activation to syngas will be presented.

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Vljudno vabljeni / Kindly invited