Univerzita Karlova v Praze, Přírodovědecká fakulta

Sekce chemie PřF UK v Praze
zve všechny zájemce na přednášku z cyklu

Quo Vadis Chemie

Understanding the Rh-Catalyzed Asymmetric 1,4-Addition by Computational Chemistry

kterou přednese

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dne 21.03. v 15:00 hod.
v posluchárně CH2, v budově chemických kateder PřF UK
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Abstrakt: Chiral compounds are of great interest to society due to their use for manufacturing of pharmaceuticals. Among various methods for making such chemicals, asymmetric catalysis is the most appealing because it also imparts synthetic efficiency and environmental friendliness. The Rh-catalyzed asymmetric 1,4-addition, first developed by Hayashi group, has become one of the most important catalytic asymmetric C-C bond forming reactions. Computational studies have the potential to reveal important details for the nature of the enantioselection process and aid new ligand design. In this lecture, modeling of the enantioselectivity for Rh/chiral diene catalysts, including the computational design of new chiral diene ligands, and investigation of the turnover-determining transmetallation step by density functional theory calculations will be presented.