



Univerzita Karlova v Praze, Přírodovědecká fakulta

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

## Quo Vadis Chemie

# Computational Design of Homogeneous Catalysts and Other Functional Organometallic Compounds



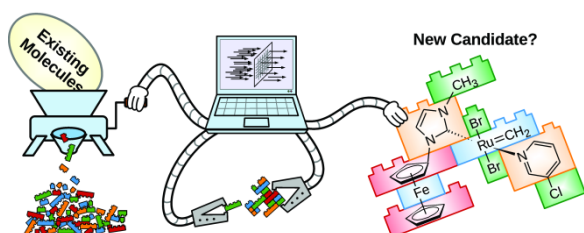
kterou přednese

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Traditional design and discovery processes in chemistry are largely driven by serendipity and improving the design usually requires costly and time-consuming experimental trial-and-error. However, little by little the tedious experiment-only approach is being replaced by experiment–theory–experiment strategies in which computational chemistry not only provides *a posteriori* insight but also is an integral part of development. The level of sophistication and automation of such combined strategies varies, ranging from computational chemistry methods used in a “manual” trial-and-error fashion to *de novo* molecular design methods that may predict new functional compounds automatically. We will focus on the methods that do not need manual intervention and in particular look at how high-quality geometries of



transition metal complexes may be automatically constructed from fragments, and how the user may control the kinds of bonds formed in this process in order to predict realistic and synthesizable molecules. Finally, examples of designed homogeneous catalysts and functional organometallic complexes will be given.