unicat
Unifying Concepts in Catalysis

Joint Colloquium:
UniCat and CRC/Transregio 63

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An Optimization-Based Method for the Design of Novel Molecular Systems

Computational molecular design (CMD) is a methodology which applies optimization techniques to develop novel lead compounds for a variety of applications. The product design framework developed in this work seeks to accelerate the commonly used experimental trial-and-error approach by searching through large molecular spaces to provide a set of chemical structures likely to match a set of desired property targets. In this presentation, an overview of CMD methods used in our group is presented.

Two major challenges are defined: the prediction of physical, chemical and biological properties of various molecular systems, and the determination of chemical structures matching a set of property targets within a large molecular space. To predict the physical and chemical properties of a specific class of molecules, quantitative structure-property relations (QSPRs) are developed which predict values of such properties as solubility, diffusivity, toxicity, polymer glass transition temperature, critical properties, and melting and decomposition temperatures.

The selection of molecular descriptors for the QSPRs is performed using Mallow's Cp statistic, which combines a goodness-of-fit score with a penalty for overfitting. The resulting property prediction models are then integrated within a computational molecular design framework, which combines the QSPRs with structural feasibility constraints in a combinatorial optimization problem. This problem is solved using a stochastic algorithm, Tabu Search, which is quite efficient for finding numerous near-optimal solutions corresponding to novel chemical structures meeting the property targets set by the designer.

Two example systems are described in this presentation: the design of novel ionic liquids (ILs) for use as refrigerants and solvents, and the development of a novel polymer mixture for dental applications.

Thursday, May 28, 2015 at 3:00 PM

Lecture Hall TK 28
TU Berlin, Building TK, Straße des 17. Juni 135, 10623 Berlin

Prof. Wozny (TUB)
Organizer

Guests are cordially invited to attend!