Forcefield-based Examinations of Interactions between Ligands and Cellulose-Surfaces and Implementation of a Web-Based Service for Interactive Calculation of Reaction-Animations of Organic Multistep Reactions

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Within the scope of this dissertation, the interactions between cellulose-surfaces and miscellaneous ligands have been examined and a web-service for the interactive generation of animations for several organic one- and multi-step reactions has been implemented.

Cellulose, the most abundant biopolymer on earth, is at all times a very important material. To modify this material by surface treatment and by this way customizing the surface for industrial requirements in an optimal way, theoretical methods and computer-simulations gain more and more importance for the predictions of molecular interaction, i.e for the question, if a given substance and surface show a desirable interaction. With this background, we have developed a method, which, by a combinations of Monte-Carlo (MC) docking and Molecular Dynamic (MD) simulations, allows positioning of ligands on a cellulose-surface and monitoring of their mobility within the time frame of the MD-simulation. We have employed a multi-stage numeric analysis-procedure, based on radial distribution functions (RDF) between ligand- and cellulose-atoms, which allows for a half-quantitative evaluation of the mobility of ligands on cellulose surface.

The visualisation of chemical reactions by computer-animations shall establish a better understanding of the course of reaction-mechanisms on a molecular level. In lectures ready-made animations are a useful tool for the lecturer to impart knowledge on reaction sequences. With iORAo [1] an interactive system has been developed for the creation of 3D-animations and also of multi-step reactions, which allows the user to interact actively with the scene by manipulating the involved molecules and by this way altering the result of the reaction outcome. This shall primarily encourage the student to study the influence of different functional groups on the reaction. iORAo is freely available via the Internet and is designed as an open platform which allows an extension of the content with additional reaction-types as well as the translation into other languages.

[1] Stueker, O. iORAo: Interactive Organic Reaction Animation Online. **http://oc24.uni-paderborn.de/iorao** (visited 2008)