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STOCHASTIC SIMULATION OF CHEMICAL WAVES USING CELLULAR AUTOMATA

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In this poster ,we present a new approach to simulate the chemical wave propagation in an excitable medium in 2D and 3D. We modified the usual cellular automata model such that wave propagation occurs only with a certain probability. In the simulations we have successfully reproduced the dynamic behaviors of the chemical waves as spherical reaction front, two-dimensional spiral evolution, wave propagation around an obstacle, and three-dimensional spiral (helix) formation. Using the stochastic approach we obtained a more realistic microscopic shape of the reaction fronts and the application of the cellular automata model resulted in a fast computational procedure. A further advantage of our approach is that the thickness of excited and refractory zones (chemical wave) can also be controlled.

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IRON COMPLEXES OF POLYDENTATE N,O-LIGANDS AND THEIR USE IN CATALYTIC OXIDATIONS

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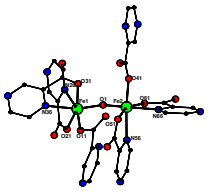
The controlled oxygenation of hydrocarbons, especially saturated hydrocarbons, catalyzed by metal complexes is one of the most important technologies for the conversion of petroleum products to useful chemicals. Because of the considerable pressure to replace old technologies with more efficient and sustainable alternatives, H_2O_2 and O_2 are among the most important oxidants for large-scale industrial applications. Since some of iron enzymes catalyze reactions as dihydrogen peroxide degradation, fatty acid oxidation or methane to methanol conversion, bio-inspired catalytic oxidations might represent a valuable approach for the development of new and more environmentally friendly catalysts.[1,2]

Efforts to model the major structural features of the hydroxylase component of the enzyme methane monooxygenase (MMO), lead to the synthesis and characterization of new iron complexes containing polydentate ligands.[3,4] The catalytic activity of these complexes for the selective oxidation of a range of substrates has been investigated. The experimental results show that the catalytic efficiency is highly dependent on the presence of additives and the reaction conditions. The stability of the catalysts, the possible active species involved in the catalytic cycle and the influence of H_2O_2 concentration on the products yield will be discussed.



The μ-oxo diiron(III) core of the compound $Na_2\{[Fe(pca)_3]_2O\}\cdot 2CH3CN\cdot 2H_2O$.

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