Combinatorial Chemistry

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Combinatorial chemistry is a state-of-the-art tool in synthetic molecular chemistry. The movement from knowledge-based discovery of synthetic strategies towards an application-based preparation of functional molecules has enabled the development of search strategies for molecules with pre-planned functions in many areas of life science, drug design, agrochemistry and materials science.

A derivative of the methodology of automated high throughput synthesis and generic functional testing has more recently been introduced into solid state materials science and heterogeneous catalysis. In proof-of-concept studies it was possible to synthesise electronic and catalytic materials which corroborated the compositional know-how empirically found earlier.

The development of truly combinatorial or evolutionary strategies in designing the experiments has made substantial progress in molecular chemistry. In solid state high throughput experiments none of these concepts have been applied yet in any meaningful complexity. Besides methodical shortcomings in instrumentation, functional testing and software development there are also fundamental barriers. In catalysis it is almost impossible to arrive at a target for a catalytic reaction, as the desired reaction is always convoluted by a large number of unknown elementary steps from which only few are relevant for the formation of the reaction product. The function of a solid often depends on its real structure which is affected by the kinetics of its genesis and not by the (thermodynamic) parameter of composition. In addition, frequent and wide miscibility gaps for components of inorganic solids exist which prevent the formation of homogeneous stable systems. Unknown chemistry and extremely difficult-to-control kinetics of synthesis lead to irreproducible solid phase mixtures and thus to the same problems as encountered in conventional empirical materials development.

The presentation will give strategic considerations and try to assess the possible merits of combinatorial methods in solid state functional material science. In heterogeneous catalysis it is difficult to foresee any fundamental breakthrough beyond a miniaturised "Mittasch" approach which may be, however, of industrial relevance.