Preface

Combinatorial methods were first introduced in chemistry, for the discovery of pharmaceutical compounds and enzymes. Later on, the application was extended to homogeneous and heterogeneous solid catalysts. In this monograph, the combinatorial development of solid catalysts is dealt with. One of the authors, Manfred Baerns, first introduced an evolutionary technique using a genetic algorithm; in this way the composition of generations of catalytic materials was established. The work was initially done in cooperation with D. Wolf, O. Gerlach (formerly Buyevskaya) and then later with P. Claus, U. Rodemerck, D. Linke, S. Moehmel and N. Steinfeld. The second author, Martin Holeňa, joined the team in order to extend and deepen the application of mathematical and computer-science methods as prerequisites for the optimisation of the composition of the catalytic materials as well as for data analysis and data mining.

All these subjects are dealt with in this monograph and they are illustrated using some relevant case studies. In the final chapter, there is a collection of abstracts taken from relevant literature, which show the progress in the field along with some conclusions and an outlook on future developments. It is anticipated that the present text will enable more efficient execution of the development of heterogeneous catalysts.

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