Computational Modeling for Homogeneous and Enzymatic Catalysis

Edited by Keiji Morokuma and Djamaladdin G. Musaev WILEY-VCH

Computational Modeling for Homogeneous and Enzymatic Catalysis

A Knowledge-Base for Designing Efficient Catalysis



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出版者:

出版时间:2008-3

装帧:

isbn:9783527318438

Here, the world's most active and productive computational scientists from academia and industry present established, effective and powerful tools for understanding catalysts. With its broad scope nitrogen fixation, polymerization, C-H bond activation, oxidations, biocatalysis and much more this book represents an extensive knowledge base for designing efficient catalysts, allowing readers to improve the performance of their own catalysts.
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