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Altri autori (Persone)	MorokumaK <1934-> (Keiji) MusaevDjamaladdin G
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Sommario/riassunto

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.