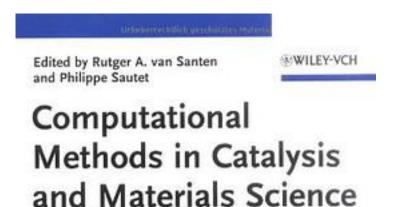
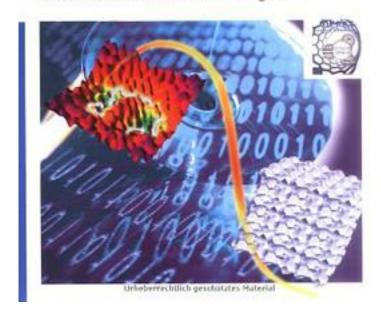
Computational Methods in Catalysis and Materials Science



An Introduction for Scientists and Engineers



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This practical guide describes the basic computational methodologies for catalysis and materials science at an introductory level, presenting the methods with relevant applications, such as spectroscopic properties, chemical reactivity and transport properties of catalytically interesting materials. Edited and authored by internationally recognized scientists, the text provides examples that may be considered and followed as state-of-the art.
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