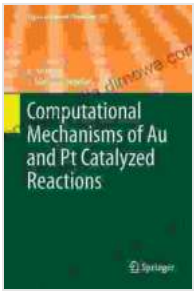
Unlock the Secrets of Au and Pt Catalysis: A Comprehensive Guide to Computational Mechanisms

Gold (Au) and platinum (Pt) are two of the most important catalysts used in a wide range of industrial and environmental processes. They are highly effective in promoting a variety of reactions, including the oxidation of carbon monoxide, the hydrogenation of alkenes, and the reforming of hydrocarbons. Understanding the mechanisms of these reactions is essential for developing new and improved catalysts. This book provides a comprehensive overview of the computational methods used to study the mechanisms of Au and Pt catalyzed reactions. It covers a wide range of topics, from the basics of density functional theory (DFT) to the latest advances in machine learning and artificial intelligence (AI).

Table of Contents

Chapter 1:

This chapter provides an overview of the book and its goals. It discusses the importance of catalysis in general, and the specific role of Au and Pt in catalysis. It also introduces the different computational methods that will be covered in the book.



Computational Mechanisms of Au and Pt Catalyzed Reactions (Topics in Current Chemistry Book 302)

by Turgon Annárë

4.3 out of 5

Language	: English
File size	: 9797 KB
Text-to-Speech	: Enabled
Screen Reader	: Supported
Enhanced typesetting	: Enabled
Print length	: 268 pages

Chapter 2: Density Functional Theory

This chapter provides a detailed overview of DFT. It covers the basic concepts of DFT, such as the Hohenberg-Kohn theorem and the Kohn-Sham equations. It also discusses the different approximations that are used in DFT, such as the local density approximation (LDA) and the generalized gradient approximation (GGA).

Chapter 3: Transition State Theory

This chapter discusses transition state theory (TST). TST is a powerful tool for understanding the mechanisms of chemical reactions. It provides a way to calculate the rate of a reaction and to identify the transition state, which is the highest energy point on the reaction pathway. This chapter discusses

the different methods that are used to calculate transition states, such as the nudged elastic band (NEB) method.

Chapter 4: Microkinetic Modeling

This chapter discusses microkinetic modeling. Microkinetic modeling is a powerful tool for simulating the behavior of catalytic reactors. It can be used to predict the conversion, selectivity, and yield of a reaction, as well as the temperature and pressure dependence of the reaction. This chapter discusses the different methods that are used to develop microkinetic models, such as the mean field approximation and the Monte Carlo method.

Chapter 5: Machine Learning and Artificial Intelligence

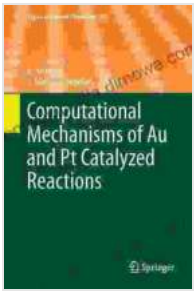
This chapter discusses machine learning and artificial intelligence (AI). Machine learning and AI are rapidly growing fields that have the potential to revolutionize many areas of science and engineering. This chapter discusses the different ways that machine learning and AI can be used to study catalysis, such as developing new catalysts, predicting reaction rates, and simulating catalytic reactors.

Chapter 6: Applications of Computational Catalysis

This chapter discusses the applications of computational catalysis. Computational catalysis is used in a wide range of industries, including the chemical, pharmaceutical, and energy industries. This chapter provides examples of how computational catalysis is used to develop new catalysts, improve existing catalysts, and design new catalytic processes.

This book provides a comprehensive overview of the computational methods used to study the mechanisms of Au and Pt catalyzed reactions. It

covers a wide range of topics, from the basics of DFT to the latest advances in machine learning and AI. This book is an essential resource for anyone who wants to understand the mechanisms of catalysis and develop new and improved catalysts.



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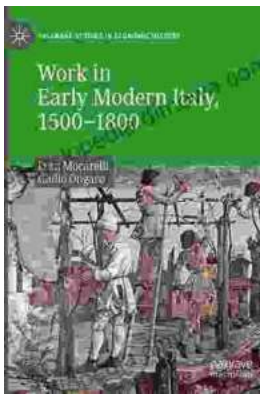

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