# Steric Effects In The Chemisorption Of Vibrationally Excited Methane On Nickel



Chemisorption is a fundamental process in surface chemistry, where a chemical species binds to a solid surface through the formation of strong chemical bonds. The understanding of chemisorption dynamics is crucial for various applications, including catalysis and surface science.

In recent studies, the chemisorption of vibrationally excited methane on nickel surfaces has attracted significant attention. Methane (CH4) is a common molecule found in natural gas, and understanding its interaction with metal surfaces is essential for developing improved catalysts for processes such as methane activation and reforming.



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Steric Effects in the Chemisorption of Vibrationally Excited Methane on Nickel (Springer

**Theses)** by Donald B. Percival (2012th Edition)

🚖 🚖 🚖 🊖 5 out of 5					
Language	: English				
File size	: 2139 KB				
Text-to-Speech	: Enabled				
Enhanced typesetting	: Enabled				
Word Wise	: Enabled				
Print length	: 397 pages				
Lending	: Enabled				
Screen Reader	: Supported				
Hardcover	: 188 pages				
Item Weight	: 1.01 pounds				
Dimensions	: 6.14 x 0.5 x 9.21 inch	es			



#### What are steric effects in chemisorption?

**Steric effects** refer to the influence of molecular size and shape on the chemical reactivity and adsorption properties of molecules. When a molecule approaches a surface, its size and shape can dictate the accessibility of its adsorption sites and the strength of intermolecular interactions.

When considering chemisorption, the steric effects become particularly interesting. Vibrationally excited methane has a higher kinetic energy and

increased molecular rotation and bending, leading to a larger spatial extension. These factors can affect the accessibility of adsorption sites on the metal surface and influence the chemisorption process.

#### The role of nickel in chemisorption

Nickel is an excellent catalyst for many chemical reactions due to its active surface sites and high reactivity. In the case of methane chemisorption, nickel acts as the surface where the molecule adsorbs and undergoes reactions.

Experimental and computational studies have shown that the adsorption of vibrationally excited methane on nickel is influenced by steric effects. The increased spatial extension of the molecule due to vibrational excitation affects the probability of the adsorption process and can lead to different reaction pathways compared to the adsorption of non-excited methane.

# Experimental techniques for studying the chemisorption of vibrationally excited methane

Understanding the complex dynamics of chemisorption requires advanced experimental techniques. Scientists use various tools to probe the interactions between vibrationally excited methane and nickel surfaces.

#### 1. Temperature Programmed Desorption (TPD)

TPD is a technique commonly used to study the desorption of adsorbed molecules from a solid surface. By ramping up the temperature, scientists can measure the desorption profiles of different molecules, allowing them to determine the reaction rates and energies involved in the chemisorption process.

#### 2. Infrared Spectroscopy (IR)

IR spectroscopy provides information about the vibrational modes of molecules. By analyzing the IR spectra of adsorbed molecules, researchers can identify the presence of vibrationally excited methane and study its interaction with nickel surfaces.

#### 3. Scanning Tunneling Microscopy (STM)

STM allows scientists to visualize individual atoms and molecules on surfaces with atomic resolution. Using STM, researchers can directly observe the adsorption of vibrationally excited methane on nickel and study the changes in surface morphology caused by the chemisorption process.

#### Implications for catalysis and surface science

Understanding steric effects in the chemisorption of vibrationally excited methane on nickel surfaces has significant implications for catalysis and surface science.

By studying the influence of molecular size and shape on the chemisorption process, researchers can design more efficient catalysts with enhanced activity and selectivity. Additionally, understanding the specific reaction pathways resulting from vibrationally excited methane adsorption can help develop strategies for controlling and optimizing methane activation and reforming processes.

The findings from these studies can also contribute to the broader understanding of chemisorption dynamics and aid in the design of materials for various applications, ranging from energy conversion to environmental remediation.

The chemisorption of vibrationally excited methane on nickel surfaces involves steric effects that influence the accessibility of adsorption sites and reaction pathways. Experimental techniques such as TPD, IR spectroscopy, and STM allow scientists to probe these interactions and gain insights into the complex dynamics of chemisorption.

Understanding steric effects in chemisorption not only advances our knowledge of surface chemistry but also has practical implications for catalysis and other applications. The further exploration of these effects could lead to the development of more efficient and selective catalysts for methane activation and contribute to the overall advancement of surface science.



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Bruce Yoder's thesis outlines his investigation of the dissociative chemisorption of methane (CH<sub>4</sub>) on a nickel single crystal. In this work Bruce uses a molecular beam and infrared laser techniques to prepare methane in excited rovibrational states. The excited methane molecules are aligned relative to the target nickel surface. Bruce describes the discovery and exploration of a previously unknown

steric effect in the dissociation reaction between a vibrationally excited methane molecule and a nickel crystal. From these studies we see that methane molecules are up to twice as reactive when the vibration is aligned parallel rather than perpendicular to the surface. This discovery will help guide the development of detailed predictive models of methane chemisorption, which in turn may lead to better catalysts for the synthesis of several industrially relevant chemicals, including hydrogen fuel from natural gas.



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