

## Accepted Manuscript

Title: Ethene hydrogenation on zeolite-supported rhodium clusters. A mechanistic study by density functional and microkinetic modeling

Authors: Velina K. Markova, Georgi N. Vayssilov, Alexander Genest, Notker Rösch



PII: S0926-860X(17)30293-4  
DOI: <http://dx.doi.org/doi:10.1016/j.apcata.2017.06.036>  
Reference: APCATA 16298

To appear in: *Applied Catalysis A: General*

Received date: 17-5-2017  
Revised date: 22-6-2017  
Accepted date: 26-6-2017

Please cite this article as: Velina K.Markova, Georgi N.Vayssilov, Alexander Genest, Notker Rösch, Ethene hydrogenation on zeolite-supported rhodium clusters.A mechanistic study by density functional and microkinetic modeling, Applied Catalysis A, General <http://dx.doi.org/10.1016/j.apcata.2017.06.036>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

# Ethene hydrogenation on zeolite-supported rhodium clusters. A mechanistic study by density functional and microkinetic modeling

Velina K. Markova,<sup>a</sup> Georgi N. Vayssilov,<sup>b</sup> Alexander Genest,<sup>a</sup> and Notker Rösch<sup>a,c,\*</sup>

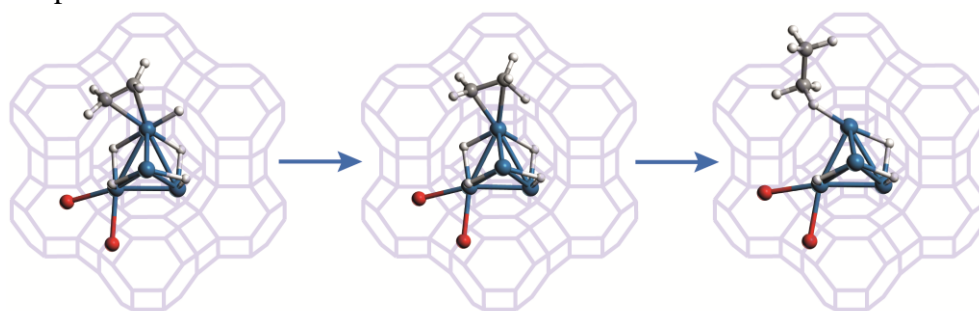
<sup>a</sup> *Institute of High Performance Computing, Agency for Science, Technology and Research, 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632, Singapore*

<sup>b</sup> *Faculty of Chemistry and Pharmacy, University of Sofia, Blvd. J. Baucher 1, 1126 Sofia, Bulgaria*

<sup>c</sup> *Department Chemie and Catalysis Research Center, Technische Universität München, 85747 Garching, Germany*

\*Corresponding author. Email: roesch@mytum.de

Graphical abstract



Hydrogenation via  $\pi$ -species

## Highlights

- Small zeolite-supported metal particles are promising candidates as catalysts in industrial processes.
- The amount of pre-adsorbed hydrogen affects the performance of small Rh particles, anchored in a zeolite, regarding the catalytic hydrogenation of ethene.
- Electronic structure calculations and microkinetic modeling show that  $\pi$ -adsorbed ethene is the active species in the hydrogenation to ethane, just as on TM surfaces.
- The coordination mode of hydrogen on TM clusters is crucial for defining the hydrogenation barriers, e.g.  $\sim 30$  kJ/mol at high H loading where weakly bound H ligands react more easily.

## Abstract

Experiments showed small Rh clusters, supported in zeolites, to be catalytically active in the hydrogenation of ethene. We report a computational study on the transformations of ethene over Rh<sub>4</sub> clusters supported in a faujasite zeolite framework, in particular on the influence of

Download English Version:

<https://daneshyari.com/en/article/4755545>

Download Persian Version:

<https://daneshyari.com/article/4755545>

[Daneshyari.com](https://daneshyari.com)