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## Title

***Furfural adsorption on V2O5 surface: A combined experimental-theoretical study***

## Abstract

The adsorption of furfural on the V2O5 surface was investigated using experimental and theoretical methods. In situ Diffuse Reflectance Infrared Fourier-Transform Spectroscopy results show the presence of physi- and chemi-sorption phenomena, where trans-furfural is mostly chemisorbed at the beginning of the adsorption process. These results are in agreement with theoretical DFT results, as the most thermodynamically favored configurations corresponds to the chemisorbed trans-furfural (T1) and cis-furfural (C1) with binding energies of  $-1.83$  and  $-2.05$  eV.

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## Authors

Lizana I.; Schott E.; Saavedra-Torres M.; Hidalgo-Rosa Y.; Pecchi G.; Karelovic A.; Zarate X.

## Author full names

Lizana, Ignacio (56803889000); Schott, Eduardo (12766226900); Saavedra-Torres, Mario (56641772000); Hidalgo-Rosa, Yoan (57210552565); Pecchi, Gina (7003407242); Karelovic, Alejandro (36166690800); Zarate, Ximena (25653306000)

## Author(s) ID

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56803889000; 12766226900; 56641772000; 57210552565; 7003407242;  
36166690800; 25653306000

## **Year**

2024

## **Source title**

Chemical Physics Letters

## **Volume**

845.0

## **Art. No.**

141288

## **DOI**

10.1016/j.cplett.2024.141288

## **Link**

<https://www.scopus.com/inward/record.uri?eid=2-s2.0-85192205328&doi=10.1016%2fj.cplett.2024.141288&partnerID=40&md5=310265808a6c225d32278d4fe1ab96>

## Affiliations

Departamento de Físico-Química, Facultad de Ciencias Químicas, Universidad de Concepción, Edmundo Larenas 129, Concepción, Chile; Departamento de Química Inorgánica, Facultad de Química y de Farmacia, Centro de Energía UC, Centro de Investigación en Nanotecnología y Materiales Avanzados CIEN-UC Pontificia, Universidad Católica de Chile Avenida Vicuña Mackenna, Santiago, 4860, Chile; Carbon and Catalysis Laboratory (CarboCat), Department of Chemical Engineering, Faculty of Engineering, University of Concepción, Concepción, 4070409, Chile; Millennium Nucleus on Catalytic Processes towards Sustainable Chemistry (CSC), Chile; Facultad de Ingeniería, Universidad Finis Terrae, Av. Pedro de Valdivia 1509, Providencia, Santiago, Chile; Instituto de Ciencias Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile Av, Pedro de Valdivia 425, Santiago, 7500912, Chile

## Authors with affiliations

Lizana I., Departamento de Físico-Química, Facultad de Ciencias Químicas, Universidad de Concepción, Edmundo Larenas 129, Concepción, Chile, Millennium Nucleus on Catalytic Processes towards Sustainable Chemistry (CSC), Chile; Schott E., Departamento de Química Inorgánica, Facultad de Química y de Farmacia, Centro de Energía UC, Centro de Investigación en Nanotecnología y Materiales Avanzados CIEN-UC Pontificia, Universidad Católica de Chile Avenida Vicuña Mackenna, Santiago, 4860, Chile, Millennium Nucleus on Catalytic Processes towards Sustainable Chemistry (CSC), Chile; Saavedra-Torres M., Millennium Nucleus on Catalytic Processes towards Sustainable Chemistry (CSC), Chile; Hidalgo-Rosa Y., Departamento de Química Inorgánica, Facultad de Química y de

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Farmacia, Centro de Energía UC, Centro de Investigación en Nanotecnología y Materiales Avanzados CIEN-UC Pontificia, Universidad Católica de Chile Avenida Vicuña Mackenna, Santiago, 4860, Chile, Facultad de Ingeniería, Universidad Finis Terrae, Av. Pedro de Valdivia 1509, Providencia, Santiago, Chile; Pecchi G., Departamento de Físico-Química, Facultad de Ciencias Químicas, Universidad de Concepción, Edmundo Larenas 129, Concepción, Chile, Millennium Nucleus on Catalytic Processes towards Sustainable Chemistry (CSC), Chile; Karelovic A., Carbon and Catalysis Laboratory (CarboCat), Department of Chemical Engineering, Faculty of Engineering, University of Concepción, Concepción, 4070409, Chile, Millennium Nucleus on Catalytic Processes towards Sustainable Chemistry (CSC), Chile; Zarate X., Millennium Nucleus on Catalytic Processes towards Sustainable Chemistry (CSC), Chile, Instituto de Ciencias Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile Av, Pedro de Valdivia 425, Santiago, 7500912, Chile

## Author Keywords

Adsorption; DFT; Furfural; In situ DRIFTS; V<sub>2</sub>O<sub>5</sub>

## Index Keywords

Adsorption; Aldehydes; Binding energy; Chemisorption; Fourier transform infrared spectroscopy; Vanadium pentoxide; Adsorption process; DFT; Experimental methods; In situ DRIFTS; Situ diffuse reflectance infrared Fourier transform spectroscopy; Situ DRIFTS; Sorption phenomena; Theoretical methods; Theoretical study; Furfural

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## Funding Details

Fondo Nacional de Desarrollo Científico y Tecnológico, FONDECYT, (1231194, ANID/FONDAP/ 1523A0006, 1241917, ACT210057, 3230141); Fondo Nacional de Desarrollo Científico y Tecnológico, FONDECYT

## Funding Texts

Funding text 1: The authors thank the financial support from the grant ANID \u2013 Millennium Science Initiative Program \u2013 NCN2021\_090, FONDECYT 1241917, FONDECYT 1231194, and ANID/FONDAP/ 1523A0006. ACT210057. ; Funding text 2: The authors thank the financial support from the grant ANID \u2013 Millennium Science Initiative Program \u2013 NCN2021\_090, FONDECYT 1241917, FONDECYT 1231194, and ANID/FONDAP/ 1523A0006. ACT210057. ANID Postdoctoral 3230141.

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## **Correspondence Address**

X. Zarate; Instituto de Ciencias Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile Av, Santiago, Pedro de Valdivia 425, 7500912, Chile; email: ximena.zarate@uautonoma.cl

## **Publisher**

Elsevier B.V.

## **ISSN**

00092614

## **CODEN**

CHPLB

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## Language of Original Document

English

## Abbreviated Source Title

Chem. Phys. Lett.

## Document Type

Article

## Publication Stage

Final

## Source

Scopus

## EID

2-s2.0-85192205328