

Accepted Manuscript

Full Length Article

A DFT study on dimethyl oxalate synthesis over Pd_{ML}/Ni(111) and Pd_{ML}/Co(111) surfaces

Bingying Han, Hao Lin, Lixia Ling, Ping Liu, Maohong Fan, Baojun Wang, Riguang Zhang

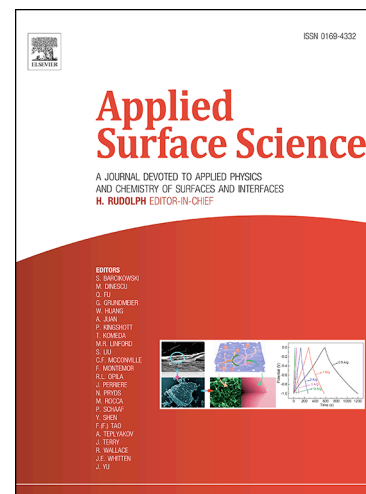
PII: S0169-4332(18)32568-6
DOI: <https://doi.org/10.1016/j.apsusc.2018.09.152>
Reference: APSUSC 40456

To appear in: *Applied Surface Science*

Received Date: 11 July 2018
Revised Date: 6 September 2018
Accepted Date: 18 September 2018

Please cite this article as: B. Han, H. Lin, L. Ling, P. Liu, M. Fan, B. Wang, R. Zhang, A DFT study on dimethyl oxalate synthesis over Pd_{ML}/Ni(111) and Pd_{ML}/Co(111) surfaces, *Applied Surface Science* (2018), doi: <https://doi.org/10.1016/j.apsusc.2018.09.152>

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.



A DFT study on dimethyl oxalate synthesis over Pd_{ML}/Ni(111) and Pd_{ML}/Co(111) surfaces

Bingying Han^a, Hao Lin^b, Lixia Ling^{*,b,c,d}, Ping Liu^c, Maohong Fan^d, Baojun Wang^{*,a}, Riguang Zhang^a

^a Key Laboratory of Coal Science and Technology of Ministry of Education and Shanxi Province, Taiyuan University of Technology, Taiyuan 030024, P.R. China

^b College of Chemistry and Chemical Engineering, Taiyuan University of Technology, Taiyuan 030024, P.R. China

^c State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan 030001, P.R. China

^d Department of Chemical and Petroleum Engineering, University of Wyoming, 1000 E University Ave, Laramie, WY 82071, USA

ABSTRACT: Pd_{ML}/Ni(111) and Pd_{ML}/Co(111) surfaces were built via Pd atoms substituting the upper one layer atoms of Ni(111) and Co(111) surfaces, and have been discussed toward dimethyl oxalate (DMO) synthesis using density functional theory (DFT) calculation and micro-kinetic modeling, which were further compared with the Pd(111) surface, in order to obtain high cost-efficiency Pd-based bimetallic catalysts. The results suggest that $\text{CO} + \text{OCH}_3 \rightarrow \text{COOCH}_3 + (\text{CO} + \text{OCH}_3) \rightarrow 2\text{COOCH}_3 \rightarrow \text{DMO}$ is the favorable route and $2\text{COOCH}_3 \rightarrow \text{DMO}$ is the rate-determining step on Pd_{ML}/Ni(111) and Pd_{ML}/Co(111) surfaces, and it is the same as that over the Pd(111) surface. The energy barriers combining with micro-kinetic modeling analysis show that the catalytic activity toward DMO synthesis follows the trend of Pd_{ML}/Co(111) > Pd_{ML}/Ni(111) > Pd(111). Moreover, DMO generation is superior to the formation of by-product DMC over Pd_{ML}/Ni(111) and Pd_{ML}/Co(111) surfaces. Therefore, Pd_{ML}/Ni and Pd_{ML}/Co bimetallic catalysts are proposed to be promising candidates for DMO formation.

Keywords: Pd_{ML}/Ni(111); Pd_{ML}/Co(111); DMO synthesis; DFT; High cost-efficiency; Activity

* Corresponding author at: No. 79 West Yingze Street, Taiyuan University of Technology, Taiyuan 030024, China. Tel.: +86 351 6010898; Fax: +86 351 6041237; E-mail address: linglixia@tyut.edu.cn (L.X. Ling); wangbaojun@tyut.edu.cn (B.J. Wang)

Download English Version:

<https://daneshyari.com/en/article/11026987>

Download Persian Version:

<https://daneshyari.com/article/11026987>

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