

Accepted Manuscript

Research paper

First-Principles Investigation of the Coupling-Induced Dissociation of Methane and its Transformation to Ethane and Ethylene

Jithin John Varghese, Bharathi Saravanan, Holger Vach, Gilles H. Peslherbe, Samir H. Mushrif

PII: S0009-2614(18)30527-X
DOI: <https://doi.org/10.1016/j.cplett.2018.06.049>
Reference: CPLETT 35748

To appear in: *Chemical Physics Letters*

Received Date: 16 March 2018
Revised Date: 19 June 2018
Accepted Date: 22 June 2018

Please cite this article as: J. John Varghese, B. Saravanan, H. Vach, G.H. Peslherbe, S.H. Mushrif, First-Principles Investigation of the Coupling-Induced Dissociation of Methane and its Transformation to Ethane and Ethylene, *Chemical Physics Letters* (2018), doi: <https://doi.org/10.1016/j.cplett.2018.06.049>

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.



First-Principles Investigation of the Coupling-Induced Dissociation of Methane and its Transformation to Ethane and Ethylene

Jithin John Varghese,^{a,1} Bharathi Saravanan,^a Holger Vach,^b Gilles H.

Peslherbe,^c and Samir H. Mushrif^{a,2,*}

^a School of Chemical and Biomedical Engineering, Nanyang Technological University, 62
Nanyang Drive, Singapore 637459

^b Laboratoire de Physique des Interfaces et des Couches Minces, CNRS UMR-7647, Ecole
Polytechnique, 91128 Palaiseau, France

^c Centre for Research in Molecular Modelling and Department of Chemistry & Biochemistry,
Concordia University, Montréal, Québec, H4B 1R6, Canada

* Email: mushrif@ualberta.ca (SHM) Ph: +1 780-492-4872 Fax: +1 780-492-2881

¹ Cambridge Centre for Advanced Research and Education in Singapore (CARES) Ltd.,
Campus for Research Excellence and Technological Enterprise (CREATE), CREATE Tower,
1 CREATE Way, Singapore 138602

² Department of Chemical and Materials Engineering, University of Alberta, 9211 - 116 St.
NW, Edmonton, Alberta, T6G 1H9, Canada

Download English Version:

<https://daneshyari.com/en/article/7837455>

Download Persian Version:

<https://daneshyari.com/article/7837455>

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