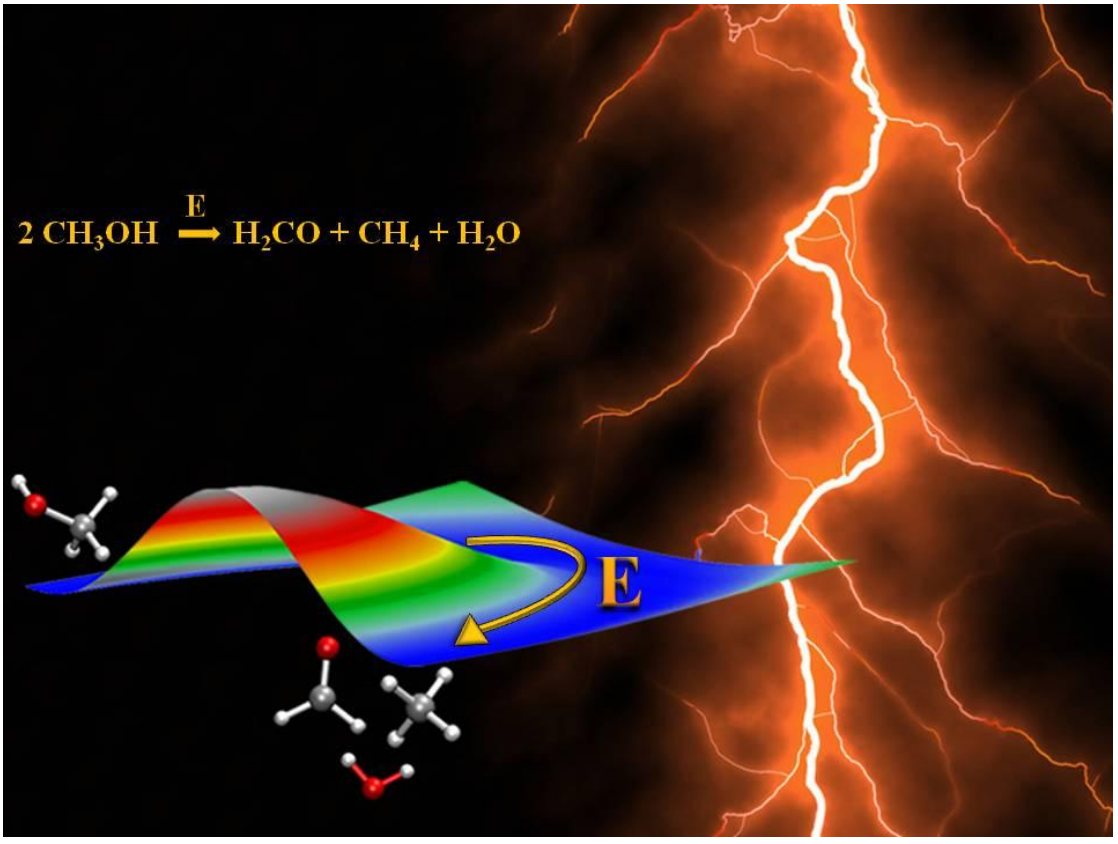
Young Minds Messina & The Optical Society OSA Messina Student Chapter


## Dr. Giuseppe Cassone

Institute of Biophysics – Czech Academy of Sciences , Brno


# *Chemical reactions driven by an electric field*




**January 24th, 2017 - Conference Room, IPCF-CNR, Messina**

**Start @ 15:30**


**Acknowledgements:**

Appunti di Fisica

CNR-IPCF

Dottorato di Ricerca in Fisica

Università di Messina

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# Chemical reactions driven by an electric field

Methanol is employed as a primary reactant in order to produce a multifaceted set of important chemical compounds, from hydrocarbons to di-hydrogen or dimethyl ether, just to cite some of the accessible derivatives. In this respect, the importance of the simplest alcohol is remarked by the envisaged possibility to base on it the world economy by the Nobel laureate G. A. Olah [1]. Among the chemical pathways that stem from methanol, formaldehyde synthesis covers a privileged role due to its manifest economic importance, but it requires the presence of specific catalysts and it is industrially achieved only in the gas phase.

*Ab initio* molecular dynamics studies have succeeded in predicting complex chemical reactions of organic molecules under extreme conditions of confinement and pressure. Moreover, the remarkable catalytic capabilities of static electric fields has been demonstrated by a series of similar quantum-based molecular dynamics investigations. However, the detailed action of the field is not understood and only very recently the first experimental evidence that electric fields are able to control chemical reactions has been provided [2].

In this talk I will present, *inter alia*, a recently published *ab initio* molecular dynamics study of liquid methanol under the effect of static electric fields [3]. It turns out that an extremely simple, but so far unreported, chemical reaction occurs at ambient temperature: $2CH_3OH \rightarrow H_2CO + CH_4 + H_2O$. This reaction has been characterized by exploiting not only the standard Density Functional Theory tools but also a newly developed scheme for the definition of efficient reaction coordinates [4] capable to reveal unexpected microscopic mechanisms and, at the same time, providing an accurate free-energy landscape, fully including the effect of the chemical environment and of the thermodynamics.


[1] G. A. Olah, A. Goeppert and G. K. S. Prakash, *Beyond Oil and Gas: The Methanol Economy*, Wiley-VCH, Winheim, Germany, 2009.

[2] A. C. Aragones, N. L. Haworth, N. Darwish, S. Ciampi, N. J. Bloomfield, G. G. Wallace, I. Diez-Perez and M. L. Coote, *Nature*, 2016, **531**, 88-91.

[3] G. Cassone, F. Pietrucci, F. Saija, F. Guyot and A. M. Saitta, *Chemical Science*, 2016, DOI: 10.1039/c6sc04269d.

[4] F. Pietrucci and A. M. Saitta, *Proc. Natl. Acad. Sci. U. S. A.*, 2015, **112**, 15030-15035.