

Methane production from H₂+CO₂ reaction without solid phase catalysis

S. Falcinelli¹, M. Rosi¹, F. Pirani², J.M. Farrar³, F. Vecchiocattivi¹

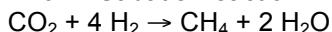
¹ Dipartimento di Ingegneria Civile ed Ambientale, Università di Perugia, 06125 Perugia, Italy

² Dipartimento di Chimica, Biologia e Biotecnologie Università di Perugia, 06123 Perugia, Italy

³ Department of Chemistry, University of Rochester, Rochester, NY 14627, USA

ABSTRACT

An open important challenge in the research field of possible strategies using low cost or renewable energy is to design and develop a heterogeneous/homogeneous catalysis processes reusing waste CO₂ to produce methane in a circular economy scheme [1]. For such a purpose is crucial to realize an optimized yield methanation stage in which hydrogen reacts with carbon dioxide to produce methane and steam water. Currently, the methanation process used in laboratory prototype apparatuses, as Progeo 20kw [1], is based on the well known Sabatier reaction



performed at high pressure (2-3 atm) and high temperature (200-300°C) with the use of a solid phase catalyst (nickel, ruthenium, or alumina).

The present contribution aims to find new efficient methanation pathways in order to avoid the use of the solid phase catalysis, exploring alternative reaction mechanisms involving the CO₂ hydrogenation through a plasma generation by electrical discharges on a CO₂+H₂ gas mixture. In order to realize this aim, the authors can employ their long expertise in modeling molecular processes (hydrogen generation, gas phase processes, molecular dynamics simulations) and in fully characterize the microscopic dynamics of elementary reactions by the experimental determination of all main kinetic parameters as rate constants, cross sections, intermolecular potentials, structure, and energy of the transition state, and related reaction pathways. Furthermore, they can conduct high resolution experiments in a single collision condition, by using crossed molecular beam apparatuses, and studying plasma induced gas phase reactions both by microwave and RF discharges [2], and by synchrotron radiation [3-5]. Such experiments are performed using the ARPES (Angle Resolved PhotoEmission Spectroscopy) end station at the GasPhase Beamline of the Elettra Synchrotron Radiation Facility (Trieste) [6,7], and the PIES (Penning Ionization Electron Spectroscopy) crossed molecular beams apparatus of the Perugia University [8,9].

REFERENCES

- [1] C. Martí, L. Pacifici, A. Capriccioli, and A. Laganà, O. Gervasi et al. (Eds.): ICCSA 2016, Part I, LNCS 9786, pp. 319–333, 2016.
- [2] B. Brunetti, D. Cappelletti, S. Falcinelli, G. Liuti, and F. Pirani, Atomic and molecular beams from electrical discharges: their characterization and applications useful for plasma diagnostic and chemical modeling. In "ISPC 12 – International Symposium on Plasma Chemistry Proceedings", Vol. 1 (1995), Ed. by J.V. Heberlein, D.W. Ernie, J.T. Roberts (Minneapolis, Minnesota, USA), pp. 343-348.
- [3] S. Falcinelli, M. Rosi, P. Candori, F. Vecchiocattivi, et al., *Planetary and Space Science* **2014**, 99, 149–157.
- [4] S. Falcinelli, F. Pirani, M. Alagia, et al., *Atmosphere* **2016**, 7, 112 1-12. DOI:10.3390/atmos7090112
- [5] S. Falcinelli, F. Pirani, M. Alagia, L. Schio, R. Richter, S. Stranges, F. Vecchiocattivi, *Chemical Physics Letters* **2016**, in press. DOI: 10.1016/j.cplett.2016.09.003
- [6] M. Alagia, C. Callegari, P. Candori, S. Falcinelli, F. Pirani, R. Richter, S. Stranges, and F. Vecchiocattivi, *J. Chem. Phys.* **2012**, 136, 204302.
- [7] S. Falcinelli, M. Alagia, J. M. Farrar, K. S. Kalogerakis, F. Pirani, et al., *J. Chem. Phys.* **2016**, 145, 114308 1-8.
- [8] S. Falcinelli, A. Bartocci, S. Cavalli, F. Pirani, and F. Vecchiocattivi, *Chemistry A European Journal* **2016**, 22, 764-771.
- [9] S. Falcinelli, M. Rosi, S. Cavalli, F. Pirani, and F. Vecchiocattivi, *Chemistry A European Journal* **2016**, 22, 12518-12526.