properties and transport coefficients starting from recent and accurate databases of atomic and molecular energy levels [1] and collision integrals [2].

Chemical equilibrium composition is a complex problem and many algorithms have been developed [3-5]. EquilTheTAis based on a new approach [6,7], which consists in solving one equilibrium equation at a time. The algorithm is based on the idea of Villars [8] soon abandoned because the original method was not easily automatized. The reaction ordering is chosen determining, at each step, which reaction is farther from equilibrium, defining a reaction distance. The algorithm is very fast and stable, finding in very few steps the concentration of principal species and refining the solution of minority species in a second stage, this feature being adequate for fluid dynamic applications. A crucial aspect is the automatic determination of a shortcut reaction that produces in a single step the same advancement resulting from hundreds of thousand steps with the original reaction set. In the calculations, Debye length and cut-off are consistently updated and virialcorrections (up to third order) can be considered.

Transport coefficients are calculated by using high order approximations of the Chapman-Enskogmethod. The Eucken [9] approximation and the Butler-Brokaw [10] equation have been used for the calculation respectively of the internal thermal conductivity and of the reactive one.

Selected results for planetary atmospheres (Earth, Mars, Jupiter) are presented.

[1] Capitelli M, Colonna G, D'Angola A, Fundamental Aspects of Plasma Chemical Physics: Thermodynamics, Vol. 66 (Springer Series on Atomic, Optical, and Plasma Physics) 2011
[2] Laricchiuta A et al. (2009) European Physical Journal D 54(3), 607
[3] Smith WR, Missen RW (1982) John Wiley and Sons, New York
[4] Meintjes K, Morgan AP (1985) Journal of Computational Physics 60, 219
[5] Reynolds W (1986) Stanford University Report ME 270 HO 7.
[6] Colonna G (2007) Computer Physics Communications 177, 493
[7] Colonna G, D'Angola A (2004) Computer Physics Communications 163, 177
[8] Villars DS (1959) Journal of Chemical Physics 60
[9] Eucken A (1913) Z. Phys. 14, 324
[10] Butler JN, Brokaw RS (1956) J. Chem. Phys. 26, 1636

#P042 - DFT investigation of polyalcohols reforming on palladium cluster

Remedios Cortese - DIpartimento di FIsica e Chimica - Università degli Studi di Palermo

Other Authors: Dario Duca, Dipartimento di Fisica e Chimica, Università degli Studi di Palermo Antonio Prestianni, Dipartimento di Fisica e Chimica, Università degli Studi di Palermo Roberto Schimmenti, Dipartimento di Fisica e Chimica, Università degli Studi di Palermo Francesco Ferrante, Dipartimento di Fisica e Chimica, Università degli Studi di Palermo

Biomass conversion technologies have recently gained high industrial interest for the production of sustainable fuels and fine chemicals; starting feedstocks for these processes are generally complex mixtures of oxygenated compounds, ranging from lignans, carbohydrates and polyalcohols to carboxylic acids [1]. Framed within this scientific context the entire reforming mechanism of two well-known polyols, namely ethylen glycol (C_2) and glycerol (C_3), on a small Pd cluster was investigated by means of density functional theory. Among the large amount of reaction pathways that can be followed in the reforming of oxygenates, we discuss here only the route that brings to carbon monoxide and hydrogen as final products, since it is the most relevant in the biomass treatment.

It was found that the C-H bond cleavage, where the H atom transfers to the cluster, has an activation energy which is typical of such processes [2] and common to all the mechanism we will deal with. On the other hand, the rate determining step (rds) is the C-C bond breaking, with an activation barrier which exceeds the 160 kJ/mol. The same investigation applied to C_3 suggests that the mechanisms of the two studied polyols cross after the C-C reforming step, through a facile 1,2 hydrogen shift in a shared intermediate.

In order to obtain information on the reforming of heavier polyols, the rds was calculated for all the stereoisomers of C_4 (erythritol), C_5 (xilytol, arabitol and ribytol), C_6 (mannitol, sorbitol, galactitol and iditol), by including the influence of the position of the breaking C-C bond. Part of the reaction mechanism is in this case affected also by secondary interaction between hydroxiles and the palladium cluster.

[1] M. Besson, P. Gallezot, C. Pinel, Chem. Rev. 2014, 114, 1827.
[2] V. D’Anna, D. Duca, F. Ferrante, G. La Manna, Phys. Chem. Chem. Phys. 2009, 11, 4077.

#P043 - Computational study of metal-free N-doped carbon networks as hydrogenation catalysts

Remedios Cortese - DIpartimento di FIsica e Chimica - Università degli Studi di Palermo

Other Authors: Francesco Ferrante (Dipartimento Fisica e Chimica Università degli Studi di Palermo), Roberto Schimmenti (Dipartimento Fisica e Chimica Università degli Studi di Palermo), Antonio Prestianni (Dipartimento Fisica e Chimica Università degli Studi di Palermo), Dario Duca (Dipartimento Fisica e Chimica Università degli Studi di Palermo)

The future development and assesment of an industry more environmental friendly will include the use of metal-free catalysts. Most of the reported metal-free catalysts are homogeneous and often their recycle is difficult; therefore, develop and