

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]. EquilTheTA is 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 virial corrections (up to third order) can be considered.

Transport coefficients are calculated by using high order approximations of the Chapman-Enskog method. 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.

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#P042 - DFT investigation of polyalcohols reforming on palladium cluster

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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 ethylene 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 (xylitol, arabitol and ribitol), 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.

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

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The future development and assessment 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

investigate them is of interest both theoretical and experimental. Recently, N-doped nanotubes and graphene sheets, were synthesized [1,2], and it was demonstrated that the incorporation, within these carbon structures, of nitrogen atoms causes a greater electron mobility and introduces more active sites for catalytic reactions. This investigation is aimed at elucidating the main features of the hydrogen fragmentation over these carbon frameworks. Several models and different theoretical approaches were employed in this investigation to characterize the structure and properties of nitrogen pyridinic moieties framed within a carbon network, commonly classified as pyridinic defects. Two different kinds of pyridinic defects configurations within a carbonaceous environment were studied. The influence of the size of the π -system and of the curvature on the ergonicity associated to the H₂ bond cleavage were analyzed. It was found that increasing the number of the benzene rings surrounding the defect the ergonicity of the reaction increases whereas the curvature of the carbon network scarcely affects this quantity.

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#P044 - UV irradiation of Methanol ice: role of the substrate

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Complex organic molecules have been detected in a lot of different astrophysical environments. Both very simple molecules like water (H₂O), carbon monoxide (CO), carbon dioxide (CO₂) and other more complex, e.g. methanol (CH₃OH), have been found in molecular clouds and hot cores (Wooden et al. 2004). However, the origin of these molecules is still controversial and many kinds of reaction pathways have been taken into account. Gas-phase reactions are not sufficient, given the low densities of the astrophysical environments. Solid-phase (ice) reactions are much more probable and can be induced by radiation. Radiation leads to the destruction of molecules, forming fragments and radicals, which in turn can react and form new, more complex, molecules. In the last decades a lot of experiments have been carried out in order to evaluate how radiation affects the ice chemical complexity. Interstellar ice analogues have been irradiated by Ultraviolet (UV) radiation and X-rays and the ice evolution has been studied. The results have given insights on the ice chemical evolution and contributed to the interpretation of the astrophysical environments. We used the Life Irradiation Facility for Exochemistry (LIFE) to irradiate a CH₃OH ice with an UV source that provides Ly- α and hydrogen molecular emission, in order to study the chemical evolution as a function of the ice thickness and the substrate composition.

#P045 - A new structural model of the human $\alpha 7$ nicotinic receptor in an open conformation.

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Nicotinic acetylcholine receptors (nAChRs) are ligand-gated ion channels that regulate chemical transmission at the neuromuscular junction [1]. Structural information is available at low resolution from an eukaryotic receptor, and at high resolution from two prokaryotic and an eukaryotic GluCl channel; and from a water-soluble homologue of the LBD of nAChRs, the pentameric acetylcholine binding protein, which has been co-crystallized with a number of agonists and antagonists [2,3].

Structures of human channels however are still lacking. Homology modeling and Molecular Dynamics (MD) simulations are valuable tools to predict structures of unknown proteins, however, for the case of human nAChRs, they have been unsuccessful in providing a stable open structure so far. On one side the homology with prokaryotic species is too low, while on the other the open eukaryotic GluCl proved itself unstable in several MD studies and collapsed to a dehydrated, non-conductive conformation, even when bound to an agonist.

In this work, we provide an all-atom structural model of the open human $\alpha 7$ nAChR in complex with the agonist epibatidine. To prevent channel closure we employ a restraint that keeps the transmembrane pore open, and obtain in this way a stable, hydrated conformation. To further validate this conformation, we run four long, unbiased simulations starting from configurations chosen at random along the restrained trajectory. The channel remains stable and hydrated over the whole runs; this allows to assess the stability of the open conformation over a cumulative time of 1 μ s, 800 ns of which are of unbiased simulation. Analysis of pore hydration and size, as well as ions distribution, interface between domains, protein hydrogen bonds network, and epibatidine conformations at the binding sites support the picture of a fully active structure both in the extracellular and transmembrane regions.