Appunti di Fisica '16
&
Dottorato di Ricerca in Fisica

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Proto-sugar synthesis via ab-initio approaches

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One of the hypothesized scenario related to the onset of life on Earth is the so-called "RNA-world". Indeed it is mostly believed that RNA occurred before DNA, basically because it could have store both genetic information and catalyzed the chemical reactions in primitive cells. This way RNA could act as a precursor of life. As it is well-known, RNA is composed of bases, phosphate groups, and ribose, this latter being one of the simplest sugars. Hence, in order to shed light on one hypothesis of the (pre)life's onset, it appears crucial to understand the most likely processes through which it has been possible to synthesize (proto)sugars. The so-called "Formose reaction" is the most known way by which, starting from an extremely simple molecule such as formaldehyde (H2CO), one can obtain ribose - and even more complex monosaccharides - by means of a series of (auto)catalytic reaction steps.

Nowadays ab initio techniques are suitable to investigate the chemical reactions that likely have led to the onset of ribose itself or to its precursors. Moreover, if these methods are joined with metadynamics approaches, one can in principle explore the energetic landscape of different reaction pathways.

We report on a series of ab initio molecular dynamics simulations that have shown to be able to reproduce part of the Formose reaction under the effect of a static electric field. Moreover, some preliminary metadynamics calculations on the formaldehyde formation from liquid methanol will be briefly presented. This way it will be possible to give some useful hints on the power of these computational techniques in predicting and/or reproducing the chemical scenarios that could have been occurred in prebiotic contexts.