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Computational Astrobiology in Bari University and ISTP-CNR

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Abstract. In this contribution, we will present some results from our latest studies in the field of computational astrobiology, which are devoted to improving our understanding of the origin and evolution of life in the Universe by means of theoretical and computational models. The phenomena that can be studied by means of numerical modeling range from the micro to the macro scale, from molecules to cosmic grains and communities of primordial organisms. These studies may help to develop a global view of the phenomena involved in the origin of life in the wider context of astrobiology.

Key words. Theoretical models – Early life simulations – Entry models – Kinetic models

1. Introduction

Astrobiology is, essentially, a multidisciplinary field, ranging from biology and chemistry, to physics and planetology. Similarly, computational astrobiology involves several disciplines: theoretical physics, plasma kinetics, biosimulations, complex system science, just to name a few.

The goal of our studies is to get a better understanding on the issue of origin and evolution of life in the Universe by using *ab initio* theoretical approaches.

In particular, the intent of the present contribution is to show how elementary processes can influence the global chemical reactions leading to the origin of the chemical species needed in the scenario of the evolution of life, in their first steps.

2. Early life simulation

One of the most interesting problems related to the origins of life is the chirality of biological molecules (Quack 2012). Our simulation algorithm is a stochastic type model, and it is based on the idea that the selection of chirality occurred due to amplified statistical fluctuations, which in turn are the result of autocatalytic processes (Longo et al. 2020).

The simulation technique has original aspects: our algorithm takes the flow of chemical energy into account, starting from energetically activated monomers of inorganic origin, up to the use of the chemical energy of the self-replication mechanism of extremely primitive living systems. The nature of the energy monomers and of the primitive life forms are not specified, for simulation purposes. The monomers can be simple sugars, or, in the light of the most recent hypotheses on primor-

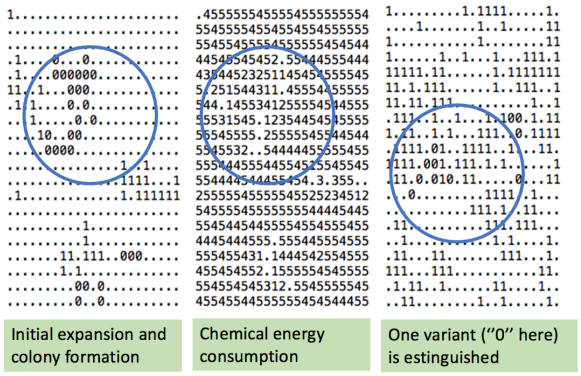

Fig. 1. Early-life simulation based on a board with periodic conditions. Two species: "0" and "1", equally fit. Here: the three stages of the process.

dial life forms, molecules containing chemical energy of different nature, such as disulfide-bonded molecules -S-S-.

Shifting the chemical selection to a stage after the origin of life, rather than before, has the advantage that the replication process itself, which is natural in a biological context, acts as an autocatalytic reaction and replaces autocatalytic processes in abiogenic contexts, which are unlikely in the context of the early Earth.

Our recently published results (Longo et al. 2020) (see figure 1) show that a chemical selection process in the context of early life forms, driven by statistical fluctuations, is possible and efficient and should therefore be taken into consideration when formulating future scenarios on the origin of life.

3. Atmospheric entry models

A critical stage of any scenario evaluating the perspective of the origin of life on Earth is the so-called delivery, *i.e.* the actual transport of molecules from space to Earth. The possibility that extraterrestrial organic matter may reach the Earth "inside" meteorites has been extensively studied in literature (Anders 1989; Chyba et al. 1990; Maurette et al. 1995; Pizzarello 2006).

In our research, we have dealt with the possibility that micrometeors carry organic matter that may have contributed to the birth of life or to its development. The study of the thermochemical behavior of micrometeoroids (MMs) entering Earth's atmosphere is of crucial interest for astrobiological science, since these objects represent ~ 90% of the total annual input of extraterrestrial matter into the biosphere (Jenniskens et al. 1998).

The innovation of our research lies in the consideration of a new composition for MMs, a new class of minerals a composition which is often associated with life forms on Earth. These materials may be collectively addressed as White Soft Minerals (WSMs) (Micca Longo et al. 2019b): they crosses the boundaries between mineralogical classifications, since this class includes carbonates, sulfates, and even organic minerals such as whewellite. Moreover, these minerals have been the subject of much research in astrobiology (see Micca Longo et al. 2019b, and references therein).

Our entry model presented comes essentially from the one developed by (Love & Brownlee 1991), but it has been extended to undertake the studies of the proposed materials (magnesite, calcite, siderite, anhydrite). All details of the model are carefully described in our works (Micca Longo & Longo 2017, 2018; Micca Longo et al. 2019a). An important aspect of the study is that WSMs, differently with respect to silicates, undergo a chem-

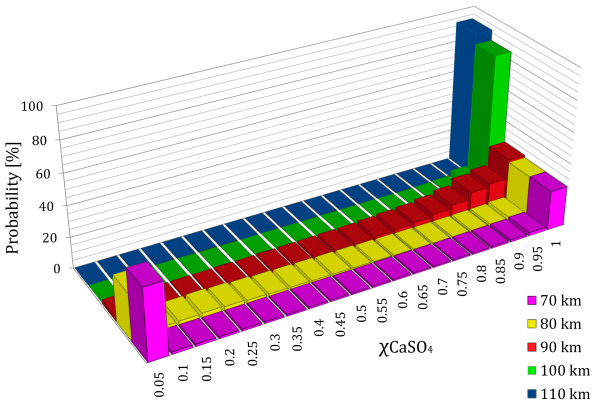

Fig. 2. Anhydrous calcium sulphate fraction occurrences at different altitudes (figure from Micca Longo et al. 2019a).

ical decomposition process at moderate temperatures (few hundreds K). This process establishes a distinction between scenarios with complete conversion of the mineral into oxide and those scenarios with partial or no decomposition. Furthermore, since it is strongly endothermic, the decomposition process may help the conservation of organic matter embedded into the inorganic matrix offered by the carbonate (Bisceglia et al. 2017).

Results of the model (see Micca Longo & Longo 2017, 2018; Micca Longo et al. 2019a) demonstrate that, among all the materials considered, anhydrous calcium sulphate is a remarkable material when testing the organic matter survival in Space and its dissemination scenario (figure 2). $CaSO_4$ can survive the atmospheric entry substantially unaltered or only partially decomposed and consequently reach the Earth's surface, and that its chemical decomposition mitigates the thermally induced damage of embedded organic matter.

The role of primordial atmospheres in the delivery of organic matter is widely discussed in (Micca Longo & Longo 2020), with results that underline how atmospheric chemical compositions may affect entry scenarios. The investigation supported by numerical calculations leads us to conclude that different chemical compositions of the upper primordial atmosphere may have actually produced very different outcomes, in terms of heating, dealing with grains passing through it.

4. Elementary processes

In order to build up a kinetic model for prebiotic chemistry, the crucial point relies on the availability of the reaction rates for the elementary processes involved in the physical system.

In recent years, studies based on R-Matrix quantum chemistry code (Tennyson 2010), and on the Local Complex Potential (LCP) model (see *e.g.* (Laporta 2017) and the references therein), led to great improvements in the quantitative understanding of the chemical reactions and in particular state-resolved cross-sections and rate coefficients have been available in literature.

Figure 3 shows, schematically, on the left hand side, the process of vibrational excitation by electron impact for a typical diatomic molecule. In particular, the figure refers to the case of a resonant collision. The quantum dynamics treatment of a resonant scattering is shown on the right hand side: the incident electron (the red arrow in the scheme) is temporarily captured by the neutral target molecule in its initial vibrational level – represented by the blue wave function "$v_i = 5$" – forming a metastable anionic state, the resonance (represented by the orange wave function). After a characteristic lifetime, the negative compound

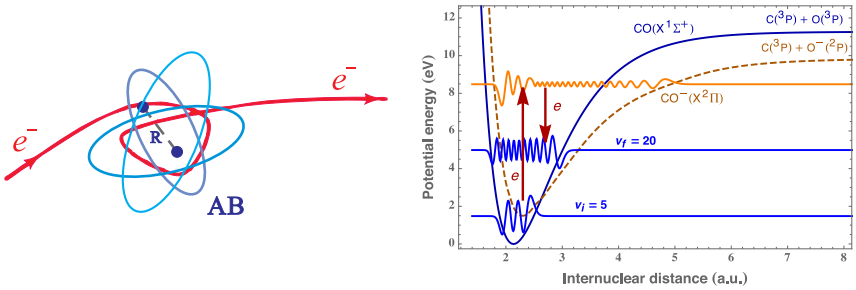

Fig. 3. (On the left) Schematic representation of a resonant vibrational excitation process by electron impact for a typical diatomic molecule. (On the right) Quantum mechanical point of view for the same process.

decays ejecting an electron and leaving the molecule in a different vibrational level (the blue wave function "$v_i = 20$").

The cross section of the full process is determined from the wave functions and the couplings between the neutral molecule and the resonant state.

The study of these elementary processes may also be important to the development of new computer models of the chemical activation of relatively inert chemical components of primordial atmospheres by energetic particles. In this way, we think that it is possible to obtain a better understanding of the biological implications of the classical experience of Miller and Urey (Micca Longo et al. 2021).

5. Conclusions

Computational astrobiology is a multidisciplinary area involving wide range of scales, from micro to macros. In this article, we showed how *ab initio* approaches can improve the understanding of scenarios of origin of prebiotic molecules and the evolution of the life in its first step.

From the short review presented here, it is clear how the range of possibilities opened by simulation models, in terms of scale and kind of physics-chemistry involved, is very wide.

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