Appunti di Fisica '18
&
Dottorato di Ricerca in Fisica

13 settembre ore 15:00
Sala seminari, CNR-IPCF

From quantum computational physics to the origins of life

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Computational approaches are nowadays a full, self-standing branch of chemistry, both for their quantum-based ("*ab initio*") accuracy, and for their multiscale extent. In prebiotic chemistry, however, due to the intrinsic complexity of the chemical problems, *ab initio* atomistic simulations have so far had a limited impact, with the exception of a few relevant studies, including the elucidation of the chemical interactions between biomolecules with surfaces, such as ice and minerals, or the simulation of the effect of the pressure/temperature shock waves induced by meteorite impacts in the early Earth. Surprisingly, even the celebrated Miller experiments, which historically reported on the spontaneous formation of amino-acids from a mixture of simple molecules reacting under an electric discharge, have never been studied at the quantum atomistic level.

Here we set the general problem of chemical networks within new topology-based concepts, using search algorithms and social network data analysis. This allows a very efficient definition of reaction coordinates even in the complex chemical environments which are typical of likely prebiotic scenarii. We thus report on the first *ab initio* computer simulations, based on quantum physics and a fully atomistic approach, of Miller-like experiments in the condensed phase. Our study [1] shows that glycine spontaneously form from mixtures of simple molecules once an electric field is switched on. We identify formic acid and formamide [2] as key intermediate products of the early steps of the Miller reactions, and the crucible of formation of complex biological molecules, as confirmed by our recent experimental and theoretical study on high-energy chemistry of formamide [3]. From a broader chemical perspective, we show that formamide plays the role of hub of a complex reaction network in both the gas and the condensed phase [4]. We are now going on a larger scale, studying the atomistic mechanisms of RNA

nucleotides synthesis [5], meteoritic amino acids [6] and sugars [7] in fully realistic prebiotic solution environments. All these results pave the way to novel computational approaches in the research of the chemical origins of life.

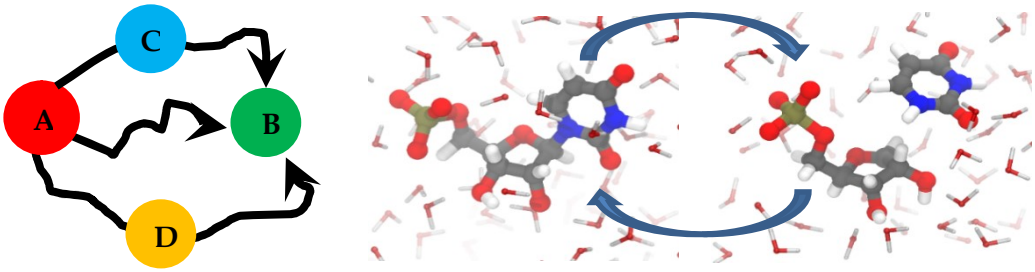

Figure 1 – Left, pictorial representation of the reaction paths connecting A and B, with possible C or D intermediates. Right, example of a fully quantum atomistic simulation of the A-to-B degradation/synthesis reaction between one uridine mono-phosphate nucleotide and one uracil plus a phosphoribose, in explicit water solution.

[1] Saitta AM and Saija F (2014) *Proceedings of the National Academy of Sciences USA* 111:13768-13773.
[2] Saitta AM, Saija F, Pietrucci F, and Guyot F (2015) *Proceedings of the National Academy of Sciences USA* 112, E343-E343.
[3] Ferus M et al. (2017) *Proceedings of the National Academy of Sciences USA*, 114:4306-4311.
[4] Pietrucci F and Saitta AM (2015) *Proceedings of the National Academy of Sciences USA* 112, 15030-15035.
[5] Perez-Villa A et al. (2018) *J. Phys. Chem. Lett.* 9, 4981–4987.
[6] Pietrucci F et al. (2018) *ACS Earth Space Chem* 2, 588-598.
[7] Cassone G et al. (2018) *Chem Comm* 54, 3211.

On the electromagnetic modes of non-Hermitian macroscopic resonators

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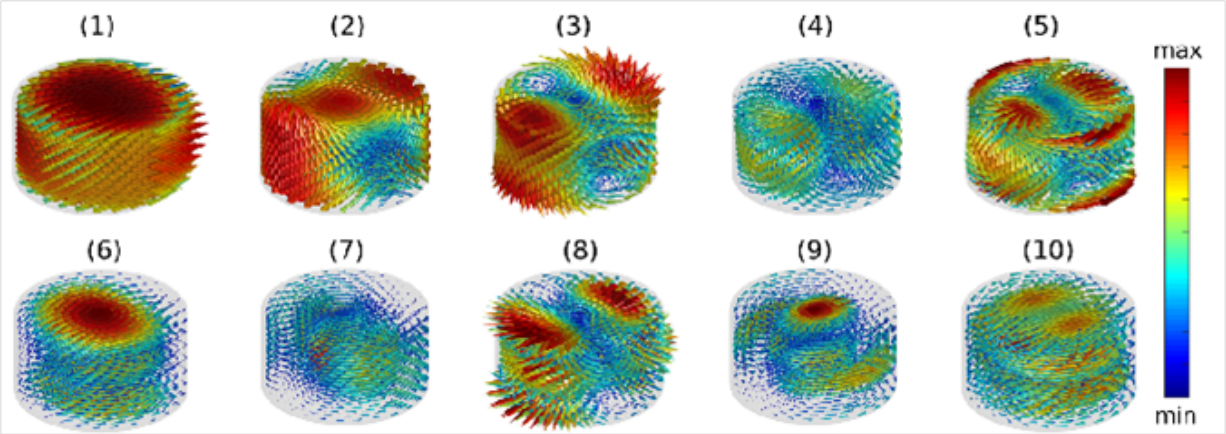
Open electromagnetic systems, such as photonic and plasmonic micro and nano-resonators, may display electromagnetic resonances, which are usually modeled by non-hermitian mathematical problems. First, I review different ways to formulate non-hermitian electromagnetic eigenvalue problems, including the quasi-normal modes (QNM) [1], and the material independent modes (MIM) [2-5]. In the QNM approach the geometry and the materials of the resonator are given, and we look for the resonator's complex resonance frequencies or "eigenfrequencies". On the contrary, in the MIM approach the geometry and operating frequency are assigned, and we look for the complex resonant permittivities or "eigenpermittivities" of the resonator. I then use each one of the aforementioned definitions to explicitly derive the resonances and the corresponding modes of an open 1D Fabry Perot resonator.

Eventually, I provide some physical insights into the MIMs representation of the electromagnetic field. Specifically, I show how this approach naturally highlights the role of plasmonic and polaritonic modes in any scattering process and suggests a straightforward methodology to design the permittivity of the object to pursue a prescribed tailoring of the scattered field.



[1] P Lalanne et al. "Light interaction with photonic and plasmonic resonances," Laser & Photonics Reviews 12 (5), 1700113 (2018).
[2] C. Forestiere and G. Miano, "Material-independent modes for electromagnetic scattering," Phys. Rev. B 94, 201406 (2016).
[3] C. Forestiere and G. Miano. "On the nanoparticle resonances in the full-retarded regime." Journal of Optics 19.7 (2017)
[4] M. Pascale, G. Miano, C. Forestiere, "Spectral theory of electromagnetic scattering by a coated sphere", JOSA B 34 (7), 1524-1535 (2017)
[5] C Forestiere et al., "Volume Integral Formulation for the Calculation of Material Independent Modes of Dielectric Scatterers" IEEE Transactions on Antennas and Propagation 66 (5), 2505-251 (2018)