

Report

"Step towards Stem Materials"

25-26 June, 2019 - Brussels

WG MATERIALS







Report of the workshop "Step towards Stem Materials"¹

Preamble: the concept of Stem Materials

In nature, living organisms consist of a limited number of primary components and chemical bonds organized in complex systems capable to adapt to diversified environmental conditions. Materials are very rarely adaptable, and often require a large number of components to achieve high performances in specific functions. In this comparison between organisms and materials, the approach to their respective life-cycles are also largely different, the former renewing in a continuous interaction with the environment, the latter mainly preserving from alterations.

Indeed, materials able to perform different functions and to respond to external inputs will become increasingly important. They will play a fundamental role in the additive production to the extent that these are designed and structured to perform specific operations and self-adapt to varying external conditions, without any additional device. This generation of materials can substitute robots in some applications, i.e. when communication and electronics are considered vulnerable aspects.

Materials able to perform as sensors and actuators, accordingly to external environmental conditions for fulfilling different requirements, are still a challenge. These intelligent materials should be flexible in any context and condition, and possibly consist of *primitive units*, containing the minimal and sufficient number of components to perform a basic function, whose *combinations* can respond to specific requests of *multi-functionality and adaptability*.

The required approach is well-known in science, looking for a bridge between the observable macroscopic and the microscopic levels, towards a coherence between descriptions of reality and complexity. It is not simply a matter of promoting inter and cross-disciplinarity, but in understanding the relationships between fundamental scientific theories and contingent conditions or environments, which can play a role in the emergence of new features.

The process to identify scientific and technological gaps

First step: Rome 2017 – scoping workshop

A the first scoping workshop was held in March 2017, when a tenth of Italian top-scientists met to exchange views and evaluate the feasibility of the concept of "Stem Materials". They identified the main aspects to be considered relevant for investigation as follows:



^{*} The adjective "stem", commonly attributed to cells, refers to the use of blocks of primitive and nonspecialized materials which, even if not able to differentiate spontaneously in several other types, undergo a process of transformation aimed to make them capable to adapt to specific requirements.





A) non-equilibrium, B) context dependency, C) multi-scale, D) cognition, E) assembling, F) synthetic biology, G) sustainability.

Second step: Rome 2018 - Face-to-Face workshop

Another workshop was organized in December 2018, and approximately 20 experts from different disciplines were asked to debate on how to pave the way and adopt action towards a general and breakthrough framework for primitive units, as a sort of ribosome of Materials and their combinations, which can enable the multi-functionality and adaptability of materials. A background document was prepared and distributed in advance to the participants, where the state of the art was reviewed.

They concluded that the following aspects have to be investigated:

the **transport/meaning of info/energy**, that is the communication flow and its language/code;

the role of **networks and scales**;

the structure and role of interfaces and non-linear elements;

the **space-time organization/dynamics** and their optimization towards the properties;

the capability to manage **multi-states systems**.

The experts also agreed in translating these challenges into a case study which can link the theory and experiments in such a way to extract knowledge. This case study has been named ABCA, which represent the simplest "logic scheme" of a stem material which transform a state A in B, then in C and coming to A again.

Towards an operational plan

Third step: Brussels 2019 - Experiments vs theoretical models

The challenges and aspects referred as relevant in the previous workshops have been already addressed in many studies on self-organizations of complex systems, in particular in addressing collective dynamics in small worlds networks or in local and global self entrainments. In this context, the role of design has still to be understood and translated into real examples.

A workshop was co-organized in cooperation with the Universitè Libre de Bruxelles, to identify some state-of-the art models which can be considered appropriate to be applied for stem materials. **Non-equilibrium systems and dynamical ordering** were at the core of the debate. Different model classes were also shown: **oscillatory/autocalytic feedback, two-step aggregation, hierarchical models**.

A proposal for the ABCA study has also been presented and the possibility to include the support of digital-twins tools has been discussed.

Finally, some experimental "dilemmas" were reported as food for thoughts, involving experienced and young researchers too.

The main outputs can be summarized as follows:

1) the awareness that mimicking nature is not the best solution, but **understanding the biological systems and multi-disciplinarity** are fundamental to proceed towards stem materials;

2) many **models are available and seem promising**: they have to be adapted to concrete examples in order to understand what theories are the appropriate to reproduce the reality;



 \square



3) the role of energy and information flows are crucial and can be treated, but indeed the synchronism between different variables is still difficult to be described and interpreted;4) a simplification in the communication of the main principles and aspects of theory is

needed: to facilitate the mutual dialogue with experimentalists and allow the use of tools in supporting visualization and clustering of concepts;

4) at least one **ABCA case study has been identified**.

References (from the workshop in Brussels)

- Bochynek T, Robson SKA (2014), "Physical and Biological Determinants of Collective Behavioural Dynamics in Complex Systems", PLoS ONE 9(4): e95112

- Gaspard P. & Kapral R. (2019) Thermodynamics and statistical mechanics of chemically powered synthetic nanomotors, Advvances in Physics: X, 4, 1

- Gaspard P. (2016) Kinetics and thermodynamics of living copolymerization processes, Phil. Trans. R. Soc. A, 374

- Gaspard P. (2013) Self-Organization at the Nanoscale Scale in Far-From-Equilibrium Surface Reactions and Copolymerizations, A. S. Mikhailov and G. Ertl, Eds., Engineering of Chemical Complexity, World Scientific, Singapore, ISBN 978-981-4390-45-3, 51-77

- Matsuda H., Ogita N., , Sasaki A., and Sato K. (1992) Statistical Mechanics of Population the lattice Lotka-volterra model, Progress of Theoretical Physics, 88, 6

- Nicolis G & Nicolis C (2005), Kinetics of phase transitions in the presence of an intermediate metastable state: A generic model, Physica A: Statistical Mechanics and its Applications 351(1):22-39

- Nicolis G. (1995) "Introduction to Nonlinear Science", Cambridge Univ. Press

- Nicolis G.& Prigogine I (1977) Self-Organization in Nonequilibrium Systems: From Dissipative Structures to Order through Fluctuations, Wiley, New York









Steps towards "Stem Materials"

25-26 June 2019 Solvay Room – Universitè Libre de Bruxelles – Campus de la Plaine, N.O. Bldg, Brussels Organized in the framework of the Science and Technology Foresight Project of the National Research Council of Italy (http://www.foresight.cnr.it/materials)

25 June - 14:00 - 18:00

Session I: Visions vs gaps

Chair: Dr. Vasileios Basios

14:00 – 14:10 Welcome: "Nonequilibrium systems: an inspiration & source of innovation" (Prof. Mustapha Tlidi, President of the Physics Dept., ULB)

 14:10 – 14:40 "Active colloidal particles: nonequilibrium dynamics and self-organization" (Prof. Pierre Gaspard, Head of Physics of Complex Systems, Dept., ULB)
 14:40 – 15:10 "The challenges of new generations of materials"

(Prof. Rodrigo Martins - UNINOVA/CEMOP)

15:10 – 15:40 "The inspiration from nature" (Prof. Olga Speck - FIT Uni Freiburg)

15:40 – 16:10 "The foresight on Stem Materials" (Dr. Pier Francesco Moretti - CNR)

16:10 – 16:30 Coffee break

Session II: Feasibility

Chair: Prof. Rodrigo Martins

16:30 – 17:00 "European vision and opportunities" (Dr. Barend Verachtert – EC DG RTD) 17:00 – 18:00 Discussion

26 June - 9:00 - 15:00

Session III: A path towards a new generation of materials Chair: Dr. Pier Francesco Moretti 09:00 – 09:15 "The Foresight on Stem materials: sprouting from Rome to Brussels" 09:15 – 09:45 "A possible idea for 'ABCA' "(Dr. Luigi Ambrosio - CNR) 09:45 – 10:25 "Possible model classes" (Dr. Vasileios Basios - ULB) 10:25 – 10:50 Coffee break

Session II: Brainstorming
Chair: Prof. Olga Speck
10:50 – 11:30 "Self-organized precipitation reactions in non-equilibrium conditions" (Dimitra Spanoudaki, Fabian Brau, Anne De Wit - ULB)
11:30 - 12:00 "The role of vesicles" (Dr. Gianfranco Peluso - CNR)
12:00 – 13:00 Discussion: The big questions on and for STEM materials
13:00 – 13:45 Light Lunch
13:45 – 15:30 Discussion: Outlook for the (near) future

