Science & Technology

FORESIGHT

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Report

"Stem Materials: clues and path identification"

12-13-14 December, 2018 - Rome

WG MATERIALS

National Research Council of Italy

Report of the F2F workshop of Foresight on Stem Materials[1]

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 the main scientific and technological gaps

In march 2017, the CNR-S&T Foresight Group on Materials and some (approximately ten) Italian scientists met to exchange views and feasibility of the concept of “Stem Materials”.
It was recognized that we are facing unprecedented impacts from simulations and processing in material sciences as well as from chemical synthetic biology, where their common approach is by trials or mimicking nature.

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* The adjective "stem", commonly attributed to cells, refers to the use of blocks of primitive and non-specialized 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.

Date of Publication: Feb 14, 2019 - referred author: pierfrancesco.moretti@cnr.it

During that "scoping" workshop, they identified the main aspects considered relevant for investigation in order to proceed:
A) non-equilibrium, B) context dependency, C) multiscale, D) cognition, E) assembling, F) synthetic biology, G) sustainability. These aspects ask for advances in physics, computational sciences, biology, chemistry. The "sustainability" carries a dual meaning: from the point of view of materials, the link with elements/critical raw materials and the end of cycle, from the point of view of biology, the concepts of homeostasis and autopoiesis.

The main dilemma remains in paving the way and adopting 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.
Based on those inputs, approximately twenty international experts accepted the invitation to join a Face-to-Face (F2F) workshop, where they were asked to discuss in detail some specific characteristic to focus on. A background document has been prepared and distributed to frame the concept and support the briefing of the participants, who were contacted one by one by phone or via email.
The F2F workshops are invitation only events, organized in such a way as to guarantee to participants from a range of backgrounds and positions the conditions necessary for a free and open debate. This approach is designed to facilitate convergence towards common positions related to research priorities, knowledge gaps and funding needs..
This F2F workshop was articulated in three days: during the first one, five experts were invited to introduce all the other participants to different issues which could be useful and probably not known by the whole community: The Materials' Genetic code, Living Materials, Non equilibrium of nanostructures, The role of chaos and rhythms in order and functioning, A whole-cell computational model: phenotype from genotype. These five talks warmed-up the multi-disciplinary debate. The second day, a first round of parallel sessions was conducted, where the composition of experts of one session was mainly composed by materials scientists. In this round, bottom-up reflections were collected and reported in the successive plenary session. A second round of parallel sessions, with mixed compositions, were guided to focus on common aspects and proposals. The outputs were reported in the last plenary session of the second day and then analyzed during the last day.

Outputs

A preliminary discussion on the complexity of Stem Materials suggested to think about them as material systems/machinery. In addition, when addressing the issue of functionality, the main principles has to be specified to identify what properties these materials should show.

The experts first identified some characteristics/aspects which are considered interesting, or challenging, and which can provide clues for a new generation of materials. In the following, these aspects are described.
a) Structure and spatial configuration is crucial for the properties and therefore for function.
b) Thresholds, interfaces, gradients, quorum sensing are all aspects linked to the relevance of non linear behavior and non-equilibrium status which characterize the adaptability and "intelligence" of Stem materials.
c) temporal fluctuations, waves and phase locking can play a fundamental role in ordering and triggering self-organization of the structures.
d) Self-replication is still an enigma to reproduce.
That said, two keywords were extracted to summarize the first round of reflections:
dynamics of processing + interfaces.

Further exchanges of view between the experts converged on some key aspects to focus the attention in running researches or future developments, as:
the **transport/meaning of info/energy**, that is the communication flow inside the system and its language/code;
the role of **networks and scales** present in the structure and in the energy/information flow;
the structure and role of interfaces and gradients, as well as the presence of non-linear elements;
the **space-time organization/dynamics** and their optimization towards the properties;
the capability to manage **multi-states systems**, which are not local in time and are dependent on the history of the process.
These aspects have been already addressed in recent studies on self-organizations of complex systems, in particular in addressing collective dynamics in small worlds networks or in local and global self entrainments, but the emerging of scaling in networks as well as the role of design has still to be understood (see references).

The experts translated their reflections into a concrete proposal which can provide breakthrough clues towards Stem Materials, and in general to any system which can be considered dynamically sustainable.
They proposed to **identify a case study** to address the simplest "logic scheme" which transform a state A in B, then in C and coming to A again (see figure 2, named for sake of simplicity **ABCA** scheme, and as the AbraCAdabra experiment!).
The states A,B,C can represent functions of the same material system or chemical compounds or whatever transformation in a closed loop.
The AbraCAdabra could be meant as a sort of **digi-twin, in the sense of validating models and theory accordingly to an experimental set-up and trials to be run**.

References

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List of annexes

Annex 1: programme of the F2F workshop (Rome, 5-7 December 2018)
Annex 2: list of participants to the workshops
Annex 3: pics of the workshops

Annex 1: Programme

Face-to-Face Workshop on "Stem Materials"
12-14 December 2018
Sheraton, Parco de' Medici Rome Hotel, Viale Salvatore Rebecchini 145, Rome, Italy

12 December – Warm-up (14:30 – 18:00)

13:00 – 14:30 Light Lunch
14:30 – 14:45 Welcome (Massimo Inguscio – President of CNR, TBC)
14:45 – 15:00 The back casting foresight approach (Ezio Andreta)
Setting the Scene (Pier Francesco Moretti)
15:00 – 16:00 Introduction to
- The Materials' Genetic code (Nicola Marzari) + Q&A
- Living Materials systems (Olga Speck) + Q&A
16:00 – 16:30 Coffee break
16:30 – 18:00 Introduction to
- Non-equilibrium of nanostructures (Bartosz Grzybowski) + Q&A
- The role of chaos and rhythms in order and functioning (Vasileios Basios) + Q&A
- A whole-cell computational model: phenotype from genotype (Maria Suarez Diez) + Q&A
18:00 – 18:15 Rules for the day after: composition of two groups.

20:00 - Dinner

13 December – Brain storming

09:00 – 11:00 Parallel sessions: open and guided discussion
11:00 – 11:30 Coffee break
11:30 – 13:00 Plenary: Report from parallel sessions and reflections
13:00 – 14:00 Light Lunch
14:00 – 16:00 Parallel sessions: open and guided discussion
16:00 – 16:30 Coffee break
16:30 – 18:00 Plenary: Report from parallel sessions and reflections

20:00 - Dinner

14 December – Suggestions

09:00 – 10:30 Points of view: commonalities and diversities
10:30 – 11:00 Coffee break
11:00 – 13:00 Suggestions towards next steps
13:00 – 14:00 Light Lunch

Annex 2: List of participants to the workshops

Surname	Name	Affiliation	Workshop 2017	Workshop 2018
Calarco	Tommaso	Juelich	1	
Camposeo	Andrea	CNR	1	1
Luisi	Pier Luigi	Swiss Fed. Institute of Technology in Zurich	1	
Ambrosio	Luigi	CNR		1
Andreta	Ezio	CNR	1	1
Arico'	Antonino	CNR	1	
Bartolucci	Cecilia	CNR		1
Basios	Vasileios	ULB		1
Casacchia	Ruggero	CNR	1	1
Cinti	Caterina	CNR		1
Del Giudice	Paolo	ISS/INFN		1
Einaudi	Giorgio	CNR	1	1
Fina	Alberto	Politecnico Torino		1
Fino	Paolo	Politecnico Torino		1
Fortunato	Elvira	CENIMAT		1
Grzybowski	Bartosz	Ulsan National Institute of Science and Technology		1
Laus	Michele	Universita' del Piemonte Orientale	1	1
Leys	Natalie	Belgian Nuclear Research Center		1
Manna	Liberato	Istituto Italiano di Tecnologia	1	
Maiorano	Vincenzo	CNR		1
Martins	Rodrigo	UNINOVA/CEMOP		1
Marzari	Nicola	École Polytechnique Fédérale de Lausanne	1	1
Molle	Alessandro	CNR	1	1
Moretti	Pier Francesco	CNR	1	1
Raucci	Maria Grazia	CNR		1
Saracco	Guido	Politecnico Torino	1	1
Saurez Diez	Maria	Wageningen University		1
Speck	Olga	FIT Uni Freiburg		1
Stellacci	Francesco	École Polytechnique Fédérale de Lausanne	1	
Vulpiani	Angelo	Universita' Sapienza Roma	1	

Annex 3: pics of the workshop