DOI: 10.1478/AAPP.99S1A34

AAPP | Atti della Accademia Peloritana dei Pericolanti
Classe di Scienze Fisiche, Matematiche e Naturali
ISSN 1825-1242

Vol. 99, No. S1, A34 (2021)

IMAGINATION IN SCIENCE: AN EXCURSUS FROM ANCIENT DEBATES TO MODERN STUDIES OF COMPLEX MATERIALS TO SUGGEST A FLIPPED CLASSROOM APPROACH

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ABSTRACT. After the Cultural Revolution in the seventeenth century, several poets believed that science was killing the beauty of art and poetry. So, imagination has been believed to be as opposite to scientific method. Fortunately, this point of view has been generally abandoned now, and the important role of imagination in science is finally well recognized. Particularly in the field of material science, the structural and dynamical properties of a system are usually unpredictable from their constituents, since they come generally from the emerging behavior of assemblies constituted by a huge number of building blocks, so imagination is indicated as an essential tool for (i) thinking experiments, (ii) interpretating their results and (iii) preparing novel materials. This makes the topic absolutely fit for a typical flipped classroom approach. Younger students may make their first knowledge of the use of imagination in science by searching for the debates taken place over the centuries: interesting stories, debates and sometimes enjoying aspects can be found, and this can surely trigger interest in the study up to the investigation of modern complex materials. Then, at school, the stories, ideas, and opinions can be consolidated under the coordination of the teacher. In this ambit, it is obvious that interdisciplinarity is a key ingredient which can surely emerge from the activities. With an eye to future perspectives, final comments and examples of modern research activity will be also reported to show how imagination can help in setting up smart procedures to prepare novel materials in modern science.

1. Introduction

1.1. Imagination in material science. The role of imagination was first analysed by van't Hoff's in 1878 (Benfey 1960). Its role can even approach that of *creativity* or even *fantasy* but must not be confused with them. Probably for most readers it may be embarrassing to deal with imagination in scientific fields since it is known that any scientific model must be subjected to the validation, well-defined experiments only are taken into account, and experiments must be repeatable. Mathematical rules and physical laws draw a scenario that may look quite rigid. This is actually the vision just after the Cultural Revolution occurred in the seventeenth century. In that period, imagination was lookd at as detrimental for arts. Furthermore, the progresses in physics and in chemistry in the last centuries allowed an unprecedentedly detailed vision of the reality: human beings cloning possibility, race to space, unprecendented electronic devices are tangible proofs that the scientific prnciples cannot be put into debeate. The idea that there is no room for imagination and creativity seems to be justified, but in reality it is only a superficial opinion. Imagination instead plays an important role in the capacity to carry out scientific research: firstly in the preparation of an experiment, secondly in the interpretation of the results of such experiments and with specific reference to material science, thirdly in the practical use of the knowledge to invent new materials and devices.

Material science has a peculiar characteristic: the smallest building blocks must be stable components of matter *i.e.*, atoms and molecules which are organized to form bigger structures. Indeed atoms are assembled to form molecules, molecules can be assembled to form supramolecular aggregates, these are organized to form macroscopic objects and devices and so on. What is peculiar is that usually a given property does not come from the properties of the building blocks but from new and unexpected emerging effects arising when such building locks are assembled toghether. This is actually well known dynamics in the physics of complex systems. It is now clear how imagination is of pivotal importance in exploiting the possibilities of having emerging properties in complex systems.

1.2. Implications in didactics. Understanding the role of imagination in material science and how researchers can use it for investigating the structure of materials is quite new for a student. Different age scholars can have different approaches of learning scientific concepts according to the extent of the argument and the depth of the subject study, always increasing with age. This makes this topic pretty fit for a complete study path across all the academic or scholar courses of study. So, all age students may first approach the development of the use of imagination in science by retrying the debates which have been taken place over the centuries. Interesting stories, debates and sometimes enjoying aspects can be found, and this can surely trigger interest in the study of modern complex materials. For this reason, a typical flipped classroom approach may be used for the younger as well as older students. Properly guided students can search for nice stories at home through standard tools for digital research, whereas at school the stories, ideas, and opinions can be consolidated under the coordination of the teacher. In this way, interdishiplinarity can emerge from the activities and, of course, group works can be also promoted in order to tickle critical thinking and idea sharing among students.

1.3. Aim of the work. For the above described reasons, herein the historical excursus from pioneering scientific works in 1600 until the modern recommendations of recent scientists is presented. This will be made in order to have a view to elaborate experiments for an active participation of students in learning. The aim of this contribution will be to give valuable information which can be used in this regard. Interdisciplinarity will be always present as a key ingredient. I hope such ideas can be useful for the curious readers to link their natural imagination-driven attitude and the rigorous world of scientific progress in material science, with the final goal to develop innovative and ever more efficient ways of teaching/learning in scholastic and academic courses.

2. Some historical background

2.1. The debate. The debate on imagination is long and certainly not new. The first comments in this sense can be traced back to around 1600. The Scientific Revolution played an important role of course: Copernicus' *"De revolutionibus orbium coelestium"* in 1543 and *"Philosophiae Naturalis Principia Mathematica"* by Isaac Newton in 1687 are important works in a framework where the mathematical/analytical approach of science was, instead, despised by a lot of poets and writers. William Blake (1757-1827), in his *Laocoon* clearly writes that the art is the tree of life, whereas the science is the tree of death; Heinrich von Kleist (1777-1811) argued that Isaac Newton would have seen, in the fascinating features of a beautiful woman, only curved lines and in her heart just its volumetric capacity. The following argument by David Herbert Richard Lawrence (1885-1930) is particularly explanatory:

> Knowledge' has killed the sun, making it a ball of gas, with spots; 'knowledge' has killed the moon, it is a dead little earth pitted with extinct craters as with smallpox; the machine has killed the earth for us, making it a surface, more or less bumpy, that you travel over (Lawrence 1930).

On the other side, John Tyndall's belief is that such common sense is just the consequence of lack in knowledge (Tyndall 1870). Tyndall's contribution to science popularization is with no doubt inestimable and it is not a case if he became a friend of Michael Faraday (1791-1867), one of the greatest experimental philosophers of all times. Although Faraday left school at the age of thirteen with, in his own words, (Thomas 1991) "little more than the rudiments of reading, writing and arithmetic", his imaginative view of the concepts, helped him to develop works "with numerous illustrations" (Faraday 2019). In contrast with the aforementioned poets, Tyndall and Faraday shared the opinion that imagination is an essential element in science.

The debate was certainly hot and in poets there was no general consensus. For example, after Isaac Newton explained the origin of the colors of the rainbow in terms of reflection of light by the minuscule water droplets dispersed in the air (Newton 1728), the poet James Thomson (1700-1748) wrote (Thomson 1727) "How just, how beauteous the refractive law" thus pointing out the importance of scientific knowledge in enhancing the beauty of Nature. John Keats (1795-1821), instead, believed that Isaac Newton destroyed the poetry of the rainbow by "reducing it to the prismatic colors" (Orel 2005). On the contrary, Richard Dawkins seemed to reinforce Thompson's point of view in the book "Unweaving the Rainbow" (1998). It is generally believed that Dawkins has said "Keats could hardly have been more wrong".

Mark Akenside (1721–1770, poet and physician) had the same opinion:

> Man loves knowledge, and the beams of truth
> More welcome touch his understanding's eye
> Than all the blandishments of sound his ear,
> Than all of taste his tongue (Akenside 1744).

as well as other popular people like the poet Hugh MacDiarmid (1892-1978) and the scientist Richard Feynman (Feynman 2011) (1918-1988).

In my opinion it is important to notice that, in this debate, a conspicuous number of people do not see science as putting poetry, human feelings and imagination at risk, but rather enhancing them. If science enhances imagination, it would be interesting to consider the vice versa *i.e.*, the effect of imagination in science, and this is the aim of the following paragraph.

2.2. The effect of imagination in science. In this regard, there are some examples of on how imagination has helped scientists in their work. I cannot but beginning by showing the peculiar case of the scientist Jacobus Henricus van't Hoff (1852-1911), the scientist who inspired this contribution. Van't Hoff was a Nobel Prize in 1901 for his studies in the physical chemistry of solutions and osmotic pressure. Well known is, in fact, the so-called "van't Hoff coefficient" (usually indicated by the letter i) indicating the effect of electrolyte dissociation in colligative properties of solutions. However, probably less known is that his first scientific intuition did not regard the chemistry of solution but, rather, the stereochemistry. During his PhD studentship, in fact, he was involved organic compounds possibility to have specific optical rotation or activity. In that period chemical formule were drawn by 2D representation on a paper sheet, a way reputed absolutely unsatisfactory by the scientist. He, instead, understanding the possibility for carbon atom to form four bonds, intuited for the first time the 3D tetrahedral distribution of chemical bonds around the carbon atom, thus justifying the existence of isomers. To be honest also Joseph Achille Le Bel (1847-1930) had the same idea more or less at the same time. Stereochemistry as discipline was officially born after Luois Pasteur's (1822-1895) observation that tartaric acid recovered from recipients for wine production was able to rotate the plane of polarized light.

Van't Hoff conjectures were published but the scientific community was against them. This happened until 1875, when the idea of atom-dependent local and specific geometries was accepted (publication "Chimie dans l'espace" - Rotterdam, 1875). After this experience, Van't Hoff held a lesson "the power of imagination in science" where he explained the important role of imagination in science. Science, in fact, has an aim, *i.e.*, to find the relationship between causes and effects and, in this search, imagination cannot but having a pivotal role. The process has therefore two steps:

i) the observation of a phenomenon: imagination is essential not only in the choice of the exact moment (and nature) of observation, but also in the choice and eventually the change of the experimental conditions of the observation in order to have a more significant inspection;
ii) the search for cause-effect relationship: in exploring the most opportune, even sometimes indirect, pathways, imagination is essential in developing hypothesis bridging the previous knowledge with the new and still to rationalize phenomena.

Van't Hoff had imagined the tetrahedral local geometry around carbon and this has been later experimentally confirmed by X-ray diffraction.

Another representative example can the lecture told by Friedrich August Kekulé (1829-1896) in 1890 in the *Benzolfest* organized in the Berlin City Hall. Aim of the meeting was to explain how carbon atoms are able to bind each other to form complex structures. That lecture was quite famous because Kekulé reported quite mythical episodes as at the origin of his theories: he declared to have hypothesized the cyclic structure of benzene after having dreamed some snakes, one of which biting its own tail to form a ring. Of course nobody knows if this really happened, but certainly Kekulé with this argument wanted to invite scientists in using imagination to develop hypothesis. It is obvious that such hypotheses must anyway be verified by rigorous tests with a scientific approach.

A third example can be given by the case of Dmitrij Mendeleev (1834-0907). He deliberately mixed his discovery of the periodic system with a legend. It is told that Mendeleev had a dream, in which he would have seen all the elements floating in the air and then landing on the table already ordered in the periodic system. After waking up, Mendeleev would have then worked hard to write down the details of his dream. As the reader can see, there is again the use of dreams to show how a discovery has been made.

These three examples show how scientists may make use of fantasy to tell their stories, but such stories can be interpreted in a slightly different, and more constructive way. Coming back to the case of Mendeleev, in his tale it tells that he worked hard to understand the exact position of the elements that's why he fell asleep, and then after waking up he worked hard to write down the scientific clues of his dream. It can be expected that the scientist has really worked hard in finding the exact order of the known elements, so this story, rather than being considered a legend, should be seen as the "real" fact *i.e.*, that the scientist has worked hard to solve the problem, both before and after the discovery. In any complex problem, imagination and intuition help, but we can interpret better Mendeleev's tale understanding the undoubted role of efforts which is parallel with that of imagination and intuition.

Like in the problem solved by Mendeleev, materials science comes out from typically many-bodies systems, characterized by countless possible configurations but with only one correct.

3. Complexity and imagination in material science

3.1. Material science for new materials. In material science the smallest building blocks are obviously atoms organizing themselves to form definite nanostructures. They usually arrange themselves into molecules but many other possibilities are present such as crystals, amorphous structures, (organic/inorganic) hybrids and so on. Such nanostructures can also arrange themselves to form macroscopic materials. This self-assembly process can have many levels. What is important to point out is that at the nanoscale, below a substance-specific size threshold, the properties of many solids becomes strongly size-dependent due to quantum size and surface effects. Surface adsorption of convenient molecules offers the stabilization of the nanostructure but also its chemical modification (functionalization) which is the first step for its piloted assembly. In summary, therefore, preparing novel materials yelds on basically three strategies:

1) the synthesis of new molecules (synthetic chemistry);
2) the blending of already known materials;
3) the reduction of the dimensionality of already known materials to the state of nanoparticles, nanowires, nanoplates.

The last strategy, in particular, takes also into account for the need of miniaturization in recent material science and nanotechnology.

These strategies are depicted in Figure 1, originating from the tree "known strategies", and can constitute different topics in physics education, with the risk of making the approach for the study or preparation of modern materials particularly dispersive and disorganized.

Of course this would be detriment for student education in academic courses. A winning and alternative approach can be the rationalization in terms of complex behavior of matter and materials. This needs imagination. Let's see why.

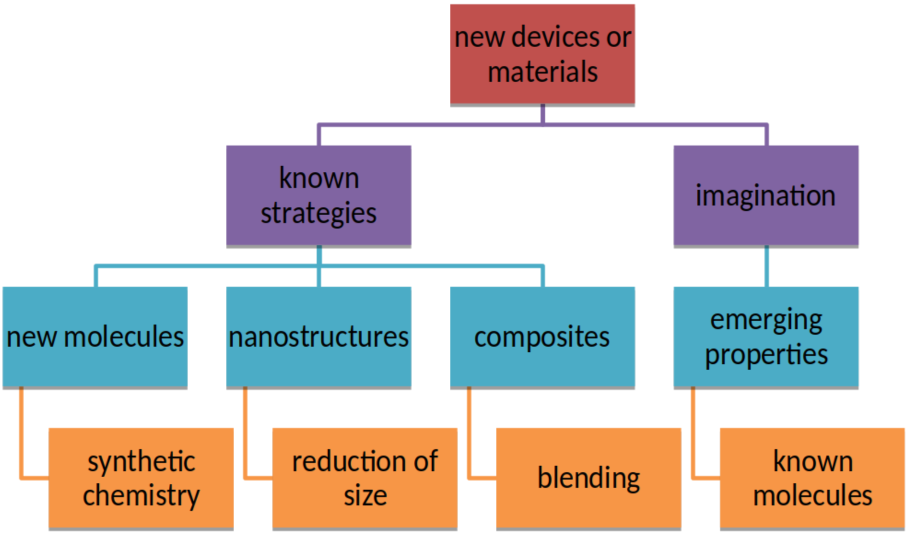

FIGURE 1. Scheme of the strategies used to build up new devices or materials in materials science.

3.2. Introducing complexity. Complexity deals with the organization of units to form bigger entities: these entities are stable if the arrangement of their sub-units is opportune. Just to introduce the topic by an example, elementary particles are somehow assembled to form atoms (physics), atoms are assembled to form molecules (chemistry), molecules can be assembled to form living cell (biology), opportunely organized living cells can constitute tissues (physiology, medicine), and so on, organs, human beings, ecosystems... in a multi-step escalation which can have a big number of levels. This is schematically depicted in Figure 2 and, from another prospect, in Figure 4.

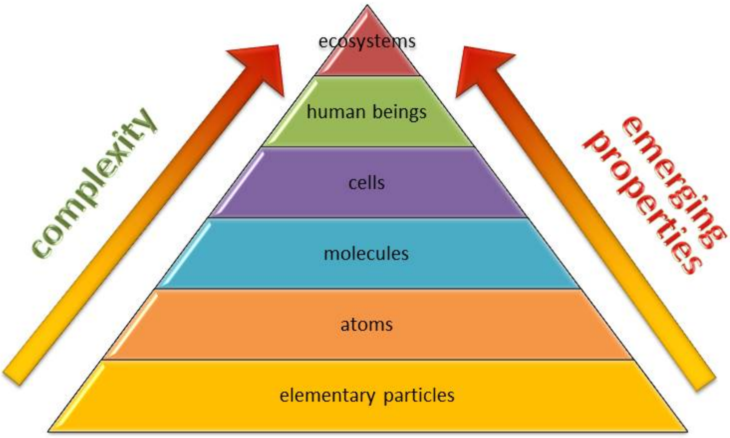

FIGURE 2. Increasing levels of complexity generate systems with emerging properties and novel functionalities.

It can be noted that that this principle is true in any kind: from chemistry to physics to sociology. If the constituents were independent and non-interacting, their assembly would be just a simple aggregation of its constituents: most of its characteristics could be predicted from the characteristics of its constituents. In this case, the assembly would have a simple behavior. Instead, if the constituents are interacting, the final assembly is not the mere collection of its building blocks and the overall properties cannot be obtained by simple extrapolation of the characteristics of their constituents: new and sometimes unexpected emerging properties can arise when passing from a level to another. In this case the systems is called to have complex behavior.

Formally, in a simple behavior an overall system property (P_l, where the subscript refers to the level of complexity labelled “l”) is the mere sum of the properties of all its i constituents obviously lying at a lower (l-1) level of complexity. (See eq. 1.)

simple system:

$$P_l = \sum_l P_{l-1}(i) \tag{1}$$

complex system:

$$P_l = \sum_l P_{l-1}(i) + f[1,2,3,\dots n] \tag{2}$$

Mass, for example, is usually a simply additive property. Instead, complex behavior arises when there are interactions among the constituents, giving a further contribution to the overall property, the contribution, shown in eq. 2, named as the function f, originating just because of the simultaneous presence of the constituents. Excess volume, for example, or any other excess property, is explicitly defined in these terms. It usually originates when two liquids are mixed, just because of the molecule-molecule interactions or even just because of different molecular sizes (Rowlinson 1971; Brandani and Prausnitz 1982).

In conclusion, the novel approach in modern materials science I want to point out is the generation of new devices/materials exploiting the emerging properties shown by the assembly of already known constituents. This approach is parallel to the aforementioned one and is reported in Figure 2, under the tree “imagination”. This approach cannot but consider imagination and intuition as the driving force.

3.3. Imagination in science. I strongly support the use of imagination in materials science. This because, readapting the idea from van’t Hoff, imagination has a fourfold role:

- helps in the choice of the exact conditions of the observation/experiment;
- the search for cause-effect relationship: in exploring the most opportune, even sometimes indirect, pathways, imagination is essential in developing hypothesis bridging the previous knowledge with the new and still to rationalize phenomena;
- it can give shortcuts in the understanding the results of the observation/experiment, by individuating cause-effect relationships which suggests new question from previous knowledge in a feedback process of ever increasing widening of knowledge;
- it can give intuition for the practical preparation of novel materials and of new devices. This is schematically depicted in Figure 3.

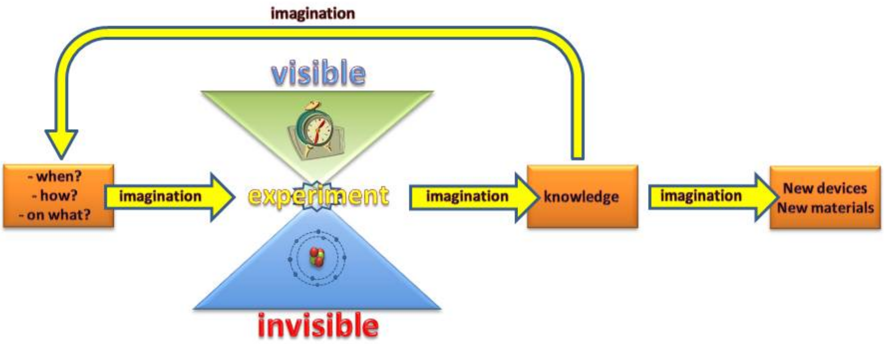

FIGURE 3. The roles of imagination is material science.

Imagination usually needs some episode to be triggered. I wil give an example: the high proton conductivity exceeding 10^{-3} S cm^{-1} at high temperatures (above 100°C) obtained by simply mixing already known materials was shown by J.D. Kim et al. in 2005 (Kim and Honma 2005). The Authors explained this emerging property in terms of two-dimensional proton-conducting pathways within the polar domains of highly ordered lamellar structures (Yamada and Honma 2004). We noticed similar effect (increase in proton conductivity) by mixing two opportunely chosen liquids (Calandra *et al.* 2010b). Driven by our belief in complex behavior importance, we imagined therefore that this peculiar effect comes from the synergy between:

- the H-bond formation;
- the intermolecular local self-assembly.

As a consequence, some surfactants can form H bonds giving availability of "mobile" protons and the consequent intermolecular self-assembly can prepare preferential pathways for their transport.
This hypothesis allowed us to prepare systems with enhanced proton conductivity (Calandra *et al.* 2012) but the idea was brought to its extremes in a quite visionary way ending up to the preparation of ionic liquids (Liveri *et al.* 2018). In fact, the coexistence of polar and apolar domains in the fluids resembles the picture of self-assembly in ionic liquids (Gowda *et al.* 2004): instead of a spatial segregation of positive and negative charges (Atkin and Warr 2008) there is a segregation of polar and apolar nano-domains. Fortunately, our hypothesis turned out to be correct and the exploitation of this effect allowed us to get, by simply mixing two opportunely chosen surfactant liquids, anomalous 1D diffusion (Calandra *et al.* 2013), exotic solubilizing properties towards inorganic salts (Calandra *et al.* 2014; Nicotera *et al.* 2014), anti-Arrhenian behavior of proton conductivity (Calandra *et al.* 2015) and even smart materials fully responsive to an external stimulus (magnetic field) (Pochylski *et al.* 2016). This can be taken as an example where imagination and the constant work inspired by the *imagined* molecular picture allowed to prepare various systems with several novel properties.

3.4. Imagination is soft materials. The same approach can be now used in an modern field of material science: *soft matter*, where the "soft" property of the structures give smart and dynamical behaviours.

Essential characteristic of the self-assembly in soft nanomaterials is the weakness of the involved forces, ususally of the order of few kJ mol^{-1} (they are called "*soft interactions*") counterbalanced by a great multiplicity of interaction sites (Hamley 2000; Shimomura and Sawadaishi 2001; Chen *et al.* 2002; Hu *et al.* 2014; Lombardo *et al.* 2018).

The localization of such strength within the framework the interactions involved at the different levels of complex systems is shown in Figure 4.

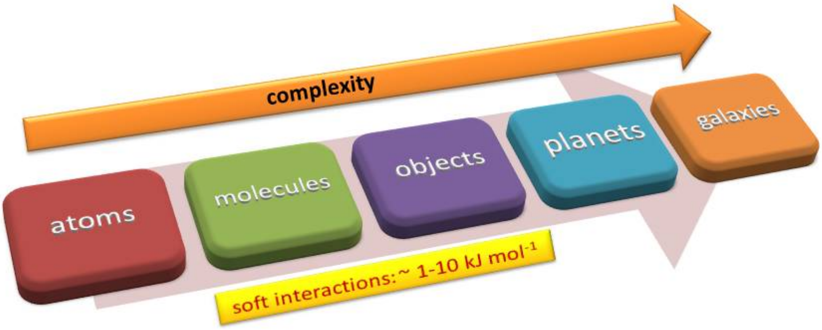

FIGURE 4. Levels of complexity in a wide lenghtscale range. The interactions strength typical of materials science is individuated.

Despite the weakness of the interactions involved, the relevant number of these forces produces, indeed, an overall effect which is strong enough to hold together different molecular structures acting as building blocks for the evolution of more complex systems (Lombardo *et al.* 2004; Whitesides and Lipomi 2009; Israelachvili 2011; Bonaccorsi *et al.* 2013a; Lombardo *et al.* 2019b).

Since a substantial change with respect to the traditional Newtonian framework is needed, a detailed treatment of the main soft (non-covalent) forces acting in nanostructures self-assembly represents a fundamental step for the understanding of the complex and cooperative behaviour in advanced functional materials (Kiselev *et al.* 2001; Mallamace *et al.* 2001; Wang *et al.* 2009; Bonaccorsi *et al.* 2013b; Menghuan *et al.* 2017). The role of soft interactions is particularly important in the constructions of nano-devices composed of heterogeneous components, as they govern the stability of component clusters, essential for the design of nanostructured materials and nanodevices (Holm *et al.* 2001; Cheng *et al.* 2006; Bonaccorsi *et al.* 2009; Lombardo 2014; Wegst *et al.* 2014).

Such interactions can be the hydrogen bonding, hydrophobic effects, polar interactions, screened electrostatic interaction, steric repulsion, van der Waals forces etc: their variety in type, strength and number of sites of interactions in multi-particles complex systems certainly require additional imaginative and creative efforts, hence crucial steps for new generation of researchers.

To this purpose, various experimental methods, from scattering (Lombardo *et al.* 2020b) to spectroscopy (Caccamo *et al.* 2020) to resonance (Calandra *et al.* 2020) better if aided by theoretical calculations/modelling techniques (Calandra 2020) can certainly help in understanding the structure of a material. This can offer different and complementary points of view, for an interdisciplinary (Lombardo *et al.* 2020a) and integrated (Lombardo *et al.* 2019a) approach. In this ambit, broader interdisciplinary scientific skills must help and integrate imagination and creativity, driving the choice of suitable models that help old problems to find the best approximate solution.

It is important to point out that soft interactions not only enhance the complexity and increase the ways in which multicomponent systems can interact, but also enlarge the range of the structural nano and meso-morphologies possible like liquids, suspensions, colloidal aggregates, biological systems (Kiselev *et al.* 2008; Howorka 2011; Kiselev *et al.* 2013; Schoonen and Hest 2015; Cohen and Louie 2016). As intruduced before, not only imagination, but also creativity, therefore, can help in modeling the complex many-body interactions, as well as the representation of the generated structured assemblies (Khokhlov *et al.* 1994; Olafsen 2010; Kiselev and Lombardo 2016; Shigemitsu and Hamachi 2017).

3.5. Imagination in nanotechnology. Finally, complex systems are pretty used in nanotechnology, another important field in material science. Nanotechnology is the controlled manipulation of matter at the nanometer scale. This control can be in space, time and/or chemical composition and can include different aspects. Already in the late '90s (Malsch 1999) it turned out that nanotechnology included nano- and quantum electronics, nanostructured materials and scanning probe microscopy, molecular materials for electronics and molecular nanotechnology, computer modelling, cluster and mesoscopic science as well as technology and supramolecular chemistry. As it can be seen, already at the very early stages of nanotechnology different fields need to be considered as part of nanotechnology and, due to the big differences among these nanotechnology must be thought as a complex structure of interconnected research areas and not as a unique field. It follows that essential aspect is the co-operation among researchers of different disciplines (interdisciplinarity), which even more, needs imagination.

For example, in a scenario where nanostructure preparation were usually carried out either by bottom-up or by top-down methods, imagination played an essential role in going beyond this distinction, so that now laser ablations (typical top-down method) of target in liquid microemulsions (whose chemical self-assembly helps in stabilizing the formation of clusters), are now well set-up methods (Calandra *et al.* 2010a, 2011) giving, as it is obvious, specific unprecedented advantages in multi-element structures (Calandra *et al.* 2010c; Trusso *et al.* 2011). Imaginative solutions sometimes start sometimes with visionary ideas, but cooperation among reserchers with interdisciplinary skills and of course hard work can bring to reality what imagination can foresee, a forefront method which cannot but being of added values in modern science.

4. Conclusions

After a debate lasted for centuries, the idea that scientists must have an imaginative attitude is quite shared now. I strongly believe that imagination plays an important role in the work of a researcher and that its crucial role in material science needs to be pointed out even from the educational and academic courses. In my opinion imagination can furnish unprecedented points of view about the way of conductiong experiments, interpreting its results, reconsider new experiments and invent new materials and devices. In this ambit, interdisciplinarity is necessary (Kaufman and Brooks 1996). In this context, and borrowing concepts from the physics of complex systems, I like to see imagination as an emerging property arising in complex research groups made by researchers with different expertises, since it inspires exchange of ideas and knowledges among people of different academic extractions. It is now advisable that the use of imagination and interdisciplinarity pass from research to education, so teaching programs should take into account for this. In this ambit, a typical flipped classroom approach may be used, where the properly guided students can search for information about the nice stories that have characterized the debates in the past, whereas at school the ideas and opinions can be consolidated under the coordination of the teacher. The development of a conceptual map is then desirable. In this way, interdisciplinarity can emerge from the activities and this can surely trigger interest up to the study of modern complex materials.

Single-discipline curricula, which have been traditionally sustained in traditional education, must be abandoned in favor of multi- and inter-disciplinary integration of knowledge and skills. This is a must, since students at any level need to have such kind of attitute for a competitive research. Apart from single-teacher interventions, a cooperative strategy is advisable: although research is already on the right way, education is unfortunately late. We wish, with this contribution, that in academic courses *ad-hoc* actions could be taken. This would give the undiscussed effect to speed up the innovation process with big advantages for future students.

Acknowledgments

Works by Prof. Vincenzo Schettino (University of Florence, Italy) have been very useful. They served as inspiration and furnished, at the same time, many useful information.

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Paper contributed to the international workshop entitled "New Horizons in Teaching Science", which was held in Messina, Italy (18–19 november 2018), under the patronage of the *Accademia Peloritana dei Pericolanti*

Manuscript received 18 May 2020; published online 30 September 2021