Compositomics: A Timely Conceptual Framework for Future Advancements in Green Materials' Design and Development

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Higher-order systems found in nature continue to be a source of inspiration for designing highly functional artificial systems. However, compositing these systems requires a precise understanding of how the components required can affect final desired responses. This non-trivial task is daunting and therefore will require a multiplicity of approaches elaborated under the umbrella of *compositomics*, a proposed –omics cluster dedicated to fabricating green materials through modeling, systems thinking, and machine learning.

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"Background of —Omics"

The history of science and engineering are intermittently punctuated by ideologic revolutions of an intensely thematic and emerging-trends nature. For example, "green chemistry," as a discipline articulated in about 1990 by John Warner and Paul Anastas, emerged from societal consciousness of industrial pollution, environmental abatement challenges, and impending petroleum-related materials and energy scarcities. Their efforts led to nucleation of work around sustainable science and engineering, industrial safety practices, green chemical engineering, biofuels, bioplastics, Life Cycle Analysis/Life Cycle Inventory, and alternative chemicals and solvents. Interestingly, major scientific concepts coalescing within a very general and encompassing new construct coined "—omics" emerged within this period. The "—omics" era was a result of systems-type thinking in biochemistry, molecular biology, and analytical chemistry that flowered in *genomics*, *transcriptomics*, *proteomics*, and *metabolomics* clusters.

All these clusters encompass collective characterization and quantification of large collections of biological molecules that translate to structure, function, and dynamics. For example, one of the fruits of genomics has been a detailed characterization of the human genome. In general, these clusters are a logical way to encapsulate a field. Interestingly, "interactomics" relates to large-scale analyses of gene-gene, protein-protein, or protein-ligand interactions. The literature has witnessed a veritable explosion of "omics" arenas since the 1990s.

Composit—omics

As a newly minted "—omics" cluster concept, not yet within the current pantheon, the "omics" that I advocate is "*compositomics*." I will take the liberty to define this as: "*a branch of the life sciences for the systematic exploration and multidisciplinary synthetic design of polymorphic (many different "shaped") systems, spanning nanoscopic to macroscopic dimensions, whose assembly and interactions lead to intelligent functionality preserved through careful assembly of the unit building blocks*". *Compositomics* does not necessarily require components to have a biochemical origin or fall under the exclusive domain of the life sciences, although that may be reasonable in modeling nature's systems. Biomimicry, a conceptual approach to modeling processes or products found in nature, is becoming a *de facto* teacher for ensuring long term and sustainable advancements in science and engineering. Therefore, it is encouraged that *compositomics* be undertaken under the guiding principle of biomimicry.

Fig. 1. A panoply of the various functionalities possible for composites (Correia *et al.* 2020)

The basis on the ideation of this cluster is to address a critical emerging need of physicists, chemists, biologists, and materials scientists to develop "smart" green composite materials, which have a multiplicity of functionality under the domain of various components whose individual functions are preserved. To date, preserved surface and bulk functions such as witnessed in cellular communication and transport processes remain under the virtually exclusive purview of nature. In addition, the photoreaction center (PRC), lignocellulosic matrices, organs/tissues, and naturally built ecosystems are "composited" in such a way to maximize function, although we cannot to date reproduce their design nor make analogous composites.

Scientists and engineers have therefore been attempting to engineer "smart" green materials using a variety of building blocks (*e.g.*, monomers, polymers, metal-inorganic complexes) that in many ways, shapes, or forms mimic nature's composite functionalities. Shown in Fig. 1 is a representation of several functional motifs available in nature whose artificial success may rely on numerous complex feedback loops and communication mechanisms. For example, actuators are systems that respond by motion and can be produced using green polymers that expand or contract as triggered by pH, electrolytes, temperature, *etc*. If we wish to incorporate green polymer-based actuators into higher-order composites that show energy storage and sensor capabilities, *etc*., then we need a detailed understanding of each component and how they can work together within a composite without compromising each one's function.

There are mathematical modeling descriptions of complex interactions within composites that consider levels and degrees of interaction among the components. They are far too complex to review here (Durai Prabhakaran *et al.* 2006), but in *compositomics*, systems theory in conjunction with these models may be reasonable.

Systems theory is a study of units or cohesive groups composed of interrelated yet interdependent parts. A system may be more than the sum of its parts if it expresses synergy or emergent behavior (Wilkinson 2011).

Finally, machine learning or more specifically artificial intelligence / fuzzy logic / neural networks may find applicability in defining and designing the complex modalities of the interactions leading to preserved function, synergy, or emergent behavior. Application of these latter computational based "machine learning" approaches is gaining acceptance in many "big data" and systems theory approaches, given the sheer volume of information and complex interrelationships among data. It may also be a part of the overall design of smart composites as a natural segue from mathematical modeling and systems thinking.

Concluding Thoughts

As the life sciences become more and more the focus of human science and engineering research, the need to organize information and data through biomimicry are becoming paramount. If we wish to simulate the elegant and very efficient natural processes listed in this editorial, we will need to adopt a *compositomics* framework. We can imagine a potential application of *compositomics* by envisioning a smart home envelope (cover) that is responsive to changes in temperature, humidity, and gases for providing optimal comfort to inhabitants. This editorial suggests several pathways to "actuate" *compositomics*. For this –omics cluster to be successful, it will need to rely on a multidisciplinary network of thinking because the complex interactions demand it.

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