Overview of Materiomics and Impact on Biological and Non-Biological Systems

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What if we could design materials that integrate powerful concepts of living organisms – self-organization, the ability to self-heal, and an amazing flexibility to create astounding material properties from abundant and inexpensive raw materials? This talk will present a comprehensive review of bottom-up analysis and design of materials for various purposes – as structural materials such as bone in our body or for lightweight composites, for applications as coatings, and as multifunctional sensors to measure small changes in temperature or stress. These new materials are designed from the bottom up and through a close coupling of experiment and powerful computation as we assemble structures, atom by atom. As a facilitator, materiomics investigates the material properties of natural and synthetic materials by examining fundamental links between processes, structures and properties at multiple scales, from nano to macro, by using systematic experimental, theoretical or computational methods [1].

We begin with a discussion of materials in biological systems, which are synthesized, controlled and used for an astonishing variety of purposes—structural support, force generation, mass transport, catalysis, or energy conversion—despite severe limitations in available energy, quality and quantity of building blocks. We show how by incorporating concepts from biology and engineering, computational modeling has led the way in identifying the core principles that link the molecular structure of biomaterials at scales of nanometers to physiological scales at the level of tissues, organs, and organisms. As a result a new paradigm of materials design has emerged, based on the insight that the way components are connected at different length-scales defines what material properties can be achieved, how they can be altered to meet functional requirements, and how they fail in disease states; rather than the chemical composition of materials alone.

The use of the world's fastest supercomputers allows us to predict properties of complex materials from first principles, realized in a multiscale modeling approach that spans massive ranges in scale, and that incorporates massive amounts of data. Combined with experimental studies, such "*in silico*" models allow us to simulate disease, understand catastrophic failure of tissues and organs, and enable us to translate concepts from the living world into groundbreaking material designs that blur the distinction between the living and non-living systems. We review case studies of joint experimental-computational work of biomimetic materials design, manufacturing and testing for the development of strong, tough and mutable materials for applications as protective coatings, cables and structural materials. We outline challenges and opportunities for technological innovation for biomaterials and beyond, exploiting novel concepts of mathematics based on category theory, which leads to a new way to organize hierarchical structure-property information. Altogether, the use of a new paradigm to design materials from the bottom up plays a critical role in advanced manufacturing, providing flexibility, tailorability and efficiency.

[1] S. Cranford, M.J. Buehler, *Biomateriomics*, 2012 (Springer, New York)