Preface

The holistic study of biological material systems has emerged as an exciting area of research. While such systems are commonly complex, we frequently encounter similar components—universal building blocks and hierarchical structural motifs—which result in a diverse set of functionalities. Similar to the way music or language arises from a limited set of musical notes and words, the relationships between form and function can be exploited in a meaningful way by recognizing the similarities between Beethoven and bone, or Shakespeare and silk. Through the investigation of material properties, examining fundamental links between processes, structures, and properties at multiple scales and their interactions, materiomics explains system functionality from the level of building blocks. *Bio*materiomics specifically focuses the analysis of the role of materials in the context of biological processes, the transfer of biological material principles towards biomimetic and bioinspired applications, and the study of interfaces between living and non-living systems. Inevitably, materiomics also holds great promise for nanoscience and nanotechnology, where material concepts from biology might enable the bottom-up development of new structures and materials or devices.

The challenges of biological materials are vast, but the convergence of biology, mathematics and engineering as well as computational and experimental techniques have resulted in the toolset necessary to describe complex material systems, from nano to macro. Applying biomateriomics can unlock Nature's secret to high performance materials such as spider silk, bone, or nacre, and elucidate the progression and diagnosis or the treatment of diseases. Similarly, it contributes to develop a *de novo* understanding of biological material processes and to the potential of exploiting novel concepts in innovation, material synthesis and design. With this impetus, the field of biomateriomics attempts to reconcile all aspects of a biological material system—from universal motifs of nano-scale building blocks to macro-scale functional properties—with a focus on studying the mechanisms of deformation and failure by utilizing a multi-scale materials science approach.

This book encompasses the current work reflective of many review articles and journal papers under a common banner, and makes this exciting field of research accessible to the broader engineering and science community. It should provide a valuable reference for engineers, materials scientists, and researchers in both academia and industry and will hopefully ignite extended discourse and inquiry. Indeed, many technical details are omitted *in lieu* of presenting key concepts and simple ideas. Many of the examples are adapted from studies carried out by the authors of this book, and some of the discussion should therefore not be considered as a comprehensive review with respect to the wider range of available results. Rather, they represent a set of specific illustrative examples of materiomics, including theoretical aspects, associated principles, and applications. The primary text provides an overview of the field of materiomics, including earlier work and future opportunities and intellectual challenges for research, and is organized into three main parts:

Part I: A Materiomics Perspective provides an introduction to biomateriomics. This is especially important given that the entire field is being developed and potential applications explored. The outside resources and investigations we henceforth refer were never intended to encompass materiomics *per se*—but yet contribute to its foundation and future progress. Admittedly, we are standing on the shoulders of others and declaring their work to be in a newfangled (and as yet unproven) field. Therein lays the stimulus for such a paradigm: only by the convergence of disparate fields can materiomics find its worth—from the astute combination of advancements in chemistry, biology, physics, materials science and engineering (further discussed in Chap. 1: Introduction). Such a combination is clearly beyond the capabilities of any individual (including these humble authors) but clearly achievable by the scientific community. The chapters constituting Part I present our interpretation of a *materiomic perspective*. The fundamental goals need only to be defined—our intent is to shed light on those goals.

For these reasons, we base this book's content around our own experience—specifically, the mechanical characterization of biological materials founded at the molecular level. We shall see that this is just one aspect of a complex *materiome*, and far from a complete picture desired (and implied) by the "omics" suffix (there is a more detailed discussion of this in subsequent chapters). Nevertheless, a focus on atomistic and molecular mechanics has various advantages:

1. It is based on fundamental principles of physics and chemistry, which are ultimately defined by quantum mechanics, providing a common starting point regardless of the specific material system(s) considered.
2. It is representative of some of the most relevant and critical topics and, most importantly, challenges in the field of biomaterials.
3. It allows us to present some case studies, which, although based on a particular scale, can easily be used as frameworks for other problems.
4. It enables other researchers to contribute to the field of materiomics, in addition to the molecular perspective emphasized here.

If our objective was to encompass all disciplines, bridge all fields, and tie together all scales of biological materials from the atomistic sequence of amino acids to a functional biological tissue or organ—we would never come to completion. Instead, we hope that through a focus on simple examples, the potential of a more holistic perspective of biological materials—discovering the relations between structure and function across multiple scales—will be apparent. As such, Part I presents the emerging field with the associated scope, thematic paradigms, and an outline of essential concepts (Chap. 2: The Materiome), as well as an in depth discussion of biological materials as the motivation for the development of a materiomics framework (Chap. 3: The Challenges of Biological Materials), and the unifying categorization and abstraction necessary for modeling and understanding such complex materiomic systems (Chap. 4: Universality-Diversity Paradigm: Music, Materiomics, and Category Theory).

Part II: Methods and Tools discusses the ever-expanding toolset required for materiomic investigations. A selection of the most promising strategies to investigate materiomics and analyze the properties and behavior of complex materials are reviewed, with examples, case studies, and theoretical background when appropriate.

In order to realize the promising opportunities that arise from an improved understanding of complex biological materials several critical challenges must be overcome. Up until now, theories fully describing hierarchical biological materials are still lacking. Only recently has the understanding about how specific features at distinct scales interact, and for example, participate in mechanical deformation, begun to emerge for complex biological systems. In recent years, the development of new quantitative experimental, analytical, and computational methods have lead to advances in understanding of some details of complex biological and synthetic systems. Theoretical, numerical, and experimental methods now enable the investigation of nanoscale mechanics of materials using quantitative analysis techniques—an area referred to as "nanomechanics". For example, development and application of nanoindentation, atomic force microscopy, and other tools enables scientist to probe the origins of mechanical properties, with forces in the range of piconewtons, and at scales approaching that of individual atoms (Ångstroms) and molecules (nanometers). At the same time, computational methods, computational power, and theoretical approaches have led to significant advances in addressing nanomechanics from a first principles perspective. This combination of experiment, theory, and computation has proven to be very fruitful, and could lead to major advances in materials theories and engineering.

The most recent innovations have occurred in the field of nanotechnology and nanoscience, where cross-disciplinary interactions with the biological sciences present an enormous opportunity for innovative basic research and also technological advancement. Such advances could enable us to provide engineered materials and structures with properties that resemble those of biological systems, in particular the ability to self-assemble, to self-repair, to adapt and evolve, and to provide multiple functions that can be controlled through external cues. However, despite significant advancements in the study of biological materials in the past decade, the fundamental physics of many phenomena in biology continue to pose substantial challenges with respect to model building, experimental studies, and simulation. As materiomics is founded by a combination of multidisciplinary theories and multiscale techniques, approaches that integrate *experiment* and predictive *simulation* are essential to this new paradigm of materials research.

The behavior of biological materials, in particular their mechanical properties, are intimately linked to the atomic microstructure of the material. Different mechanisms operate at larger length scales, where the interaction of extracellular materials with cells and of cells with one another, different tissue types and the influence of tissue remodeling become more evident. The dominance of specific mechanisms is controlled by geometrical parameters, the chemical nature of the molecular interactions, as well as the structural arrangement of the protein elementary building blocks, across many hierarchical scales, from nano to macro. Thus, materiomic investigative approaches must also consider multi-scale schemes, both experimentally and computationally, to link hierarchical effects and mechanisms.

Much of the functionality that biological materials provide occurs through mechanical contact and behavior. Therefore, to completely understand the structure-property-functionality relationships of biological materials it is necessary to quantify the mechanical behavior and influences on biological and *de novo* materials. Thus, Part II includes the means of mechanical investigation, including experimental methods (Chap. 5: Experimental Approaches), computational methods (Chap. 6: Computational Approaches and Simulation), and the interpretation of results (Chap. 7: Mechanical Characterization in Molecular Simulation). Although descriptions of techniques are to be presented, with relevant case studies and applications, specific technical details (*i.e.*, application of molecular dynamics) are only outlined, with commentary of strengths and weaknesses of various approaches, and their applicability at different scales. When appropriate, suggestions will be made for more detailed texts and references in the field. In other words, the objective of the text is not to provide an in-depth handbook for analytical procedures, but rather to discuss the various means of biomateriomic investigation. As anticipated, biomateriomics requires an extensive "toolbox".

Part III: Applied Materiomics illustrates how we can immediately benefit from biomateriomic approaches. Application of materiomic principles and approaches has already been undertaken on a variety of biological systems throughout different fields of research. The combination of high-level structural control of matter as achieved in nanoscience and nanotechnology, multiscale analytical techniques, and integration of living and non-living components into systems and interfaces will lead to the development of new technologies that utilize the advantages of both micro and nanotechnology with the principles of biology. With an inevitable merger of material and structure, with increasing complexity, materials start to resemble dynamic systems or machines, so that the borderlines between conventional concepts such as "machine" and "material" also start to disappear. Such approaches have been used systematically by Nature for millions of years. However, their systematic exploitation for technological applications has so far been severely hindered due to lack of understanding of how to link the atomistic scale with material structure and device properties and function. Like all endeavors, we only get better with practice!

Part III discusses practical applications of materiomic techniques and approaches with three main focuses. Fundamentally, materiomics provides an integrated and holistic approach, advantageous in the investigation of complex biological material system phenomenon and system characterization (Chap. 8: Unlocking Nature: Case Studies). Moreover, materiomics can facilitate the development of novel diagnostic tools for disease and afflictions with mechanistic symptoms, predicting what components and functionalities "fail" under minute changes in material and structural conditions (Chap. 9: Pathological Materiomics). Finally, biomateriomics has a role in the design of *de novo* materials, or the synthesis and manipulation of biological materials, materiomic engineering, and nanomedical devices (Chap. 10: Synthesis and Design). Using natural processes as a guide, substantial advances have already been achieved at the interface of nanomaterials and biology.

Irrespective of the challenges still present in a thorough investigation and complete characterization of the materiome as discussed by prior chapters, current experimental and practical approaches exist that allow the immediate application of materiomics to real problems. This branch of materiomics, termed *applied materiomics*, is still in its infancy, yet has already demonstrated potential as a valuable basis for material design. A materiomic approach is likely to become an integral part of nanomaterials manufacture—where molecular assembly is control to attain macroscale behavior—requiring a deep understanding of individual molecular building blocks, their potential structures, assembly properties, dynamic behavior, and multiscale propagations. We hence focus discussion on broad areas of application that are becoming increasingly widespread (throughout different disciplines) and can be encompassed by the common field of applied materiomics. The applications, undoubtedly, are as variegated as Nature. The text is closed with an outlook to future opportunities in Chap. 11: The Future of Biomateriomics.

The discussions presented in this book are intended to be both a review of current materiomics research as well as a pedagogical discourse. While we embrace the term to encompass our own work, we believe the worth of materiomics will naturally emerge from the shared contributions of many scientists and research groups. It is not a term to lay claim, but a label to encompass a new perspective of chemistry, biology, and materials science. Indeed, any "closed-form" interpretation of materiomics will limit both the growth and potential of materiomics research. As biomateriomics is a relatively new field, it behooves us to include discussion to help define and explicate both the intent and scope with analogous examples, illustrating the integrative nature, universality, and benefits and impact of a materiomics approach. The perspectives and overviews presented throughout this book are intended to provide a broad overview. Further details can be found in the papers cited and recommended readings.

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