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Bottom-up molecular models of hierarchical mineralized tissues: Structure, mechanics, biology

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Biological materials are intriguing examples of advanced materials, which are synthesized, controlled and used for an astonishing variety of purposesstructural support, force generation, mass transport, catalysis, or energy conversion. 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 macroscopic scales through hierarchical structures. Here we review case studies of a range of mineralized tissues, focused on bottom-up models and analyses of the structure and mechanics of mineralized tissues. We report an atomistic model of collagen, bone and describe the process of mineralization and the interplay of different hierarchical levels. Combined with experimental studies, such *in silico* models allow us to simulate disease, understand catastrophic failure of tissues, and enable us to translate concepts from the living world into material designs that blur the distinction between the living and non-living systems.