Toward Bioinspired Dynamic Materials Using Molecular Modeling

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Many natural materials express fascinating dynamic properties and complex functionalities that are impossible for common technological materials. These are supramolecular polymers (*e.g.*, fibers, tubes, vesicles, to name a few) built via the self-assembly of fundamental building blocks such as proteins, lipids, peptides, etc. Learning *a priori* how to design artificial materials with similar dynamic, adaptive and stimuli-responsive properties according to the same principles would be a breakthrough in many fields (1). However, the design rules to control such bioinspired dynamic properties are prohibitively difficult to catch by the experiments.

We combine multiscale molecular models (atomistic (2) and coarse-grained (3)), advanced simulation approaches and machine learning to access the intrinsic dynamics (dynamic exchange of monomers) (4) and dynamic properties of supramolecular assemblies at a sub-molecular resolution (5). This permits us to study the molecular factors that control how much and how fast/slow an assembly responds to specific stimuli (6), and to investigate at unprecedented resolution how complex self-assembled systems behave, or evolve, out-of-equilibrium (7). The scientific advance that can be obtained holds a great potential toward the rational design of next-generation dynamic materials for various technological applications.

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