Into Dynamic Supramolecular Materials at Submolecular Resolution 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 how to design artificial materials possessing similar self-healing, 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 dynamic bioinspired properties are prohibitively difficult to grasp by the experiments.

Recently, we have developed atomistic[2] and coarse-grained[3] models that allow studying the self-assembly and the properties of supramolecular polymers from a privileged point of view. Using advanced simulation approaches, we can access the intrinsic dynamics of the supramolecular polymer (dynamic exchange of monomers) at remarkably high (sub-molecular) resolution.[4] In this way, we can investigate the molecular factors that control bioinspired properties such as the ability to self-heal, or the dynamic adaptivity and stimuli-responsiveness of these materials,[5,6] We can also study out-of-equilibrium supramolecular systems.[6] The scientific advance that can be obtained opens the way toward the rational design of next-generation dynamic materials for various technological applications.

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