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Preface: Special Topic on Coarse Graining of Macromolecules, Biopolymers, and Membranes

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This special issue highlights new developments in theory and coarse-graining in biological and synthetic macromolecules and membranes. Such approaches give unique insights into the principles and design of the structures, dynamics, and assembly processes of these complex fluids and soft materials, where the length and time scales are often prohibitively long for fully atomistic modeling. © *2015 AIP Publishing LLC.* [http://dx.doi.org/10.1063/1.4938430]

Theory and coarse-grained modeling has a long and successful history in science. When Newton discovered the laws of gravity, his reasoning about apples was at the level of a point particle or a hard sphere, neither at the level of the pulp and skin and stem nor at the level of its cells or molecules. Such abstractions have been powerful across a spectrum from continuum elasticity theory of beams and shells, to the Navier-Stokes theory of fluid flow. In recent years, "coarse" has shifted to ever smaller scales, to the mesoscopic micro and nano levels.

The essential idea is to focus on a small number of relevant degrees of freedom and ignore the finer details. Often the magic is in knowing how to draw this line. Sometimes the magic is in knowing that no line can be drawn at all. In the world of biological and synthetic macromolecules, many properties have not yet yielded to coarse-graining. Examples include the folding and some functioning of proteins, such as ligand binding affinities, or the light absorption and proton transport in bacteriorhodopsin. Even so, macromolecules are often not only relevant as single entities but they can interact with each other, are often embedded in a fluid medium, and can react to changes in their environment. In such cases, the number of degrees of freedom becomes enormous and is (and will be) beyond the modeling capacities of even the largest supercomputers. Then, coarse-grained modeling may still apply in powerful ways.

Coarse graining and theory serve many useful roles. By choosing how to partition the "relevant" from the "irrelevant" degrees of freedom, we can learn about what matters. Where it gives us analytical results, it allows us to explore the dependences on variables in an efficient and informative way. It often gives more actionable insights into principles than more detailed modeling can give. And, of course, it can often turn otherwise hugely challenging modeling problems into more manageable ones.

We are truly delighted to have received such an impressive collection of papers of the highest caliber. This special issue of *The Journal of Chemical Physics* gives a flavor of the breadth and excitement and interdisciplinarity of the business of theory and coarse-graining in molecular materials. We hope you enjoy it.

