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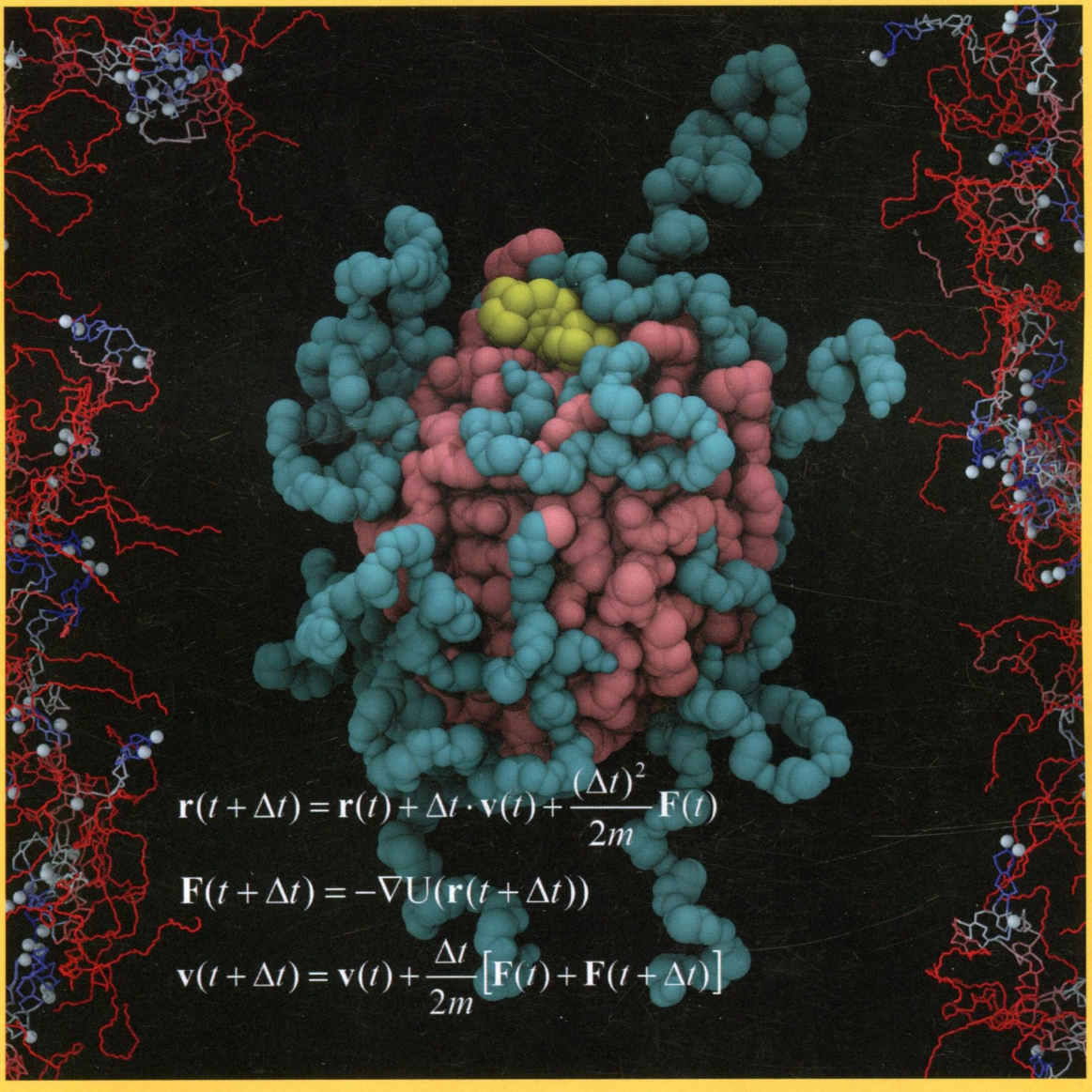

WILLIAM C. SWOPE FESTSCHRIFT

Molecular Dynamics Simulations of Drug Binding to a Star Polymer, and Polymer Synthesis

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER

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ON THE COVER: Molecular dynamics simulations of drug binding to a star polymer, and polymer synthesis. The cover shows three graphic elements. The equations describe the velocity Verlet algorithm (see: Swope, W. C.; Andersen, H. C.; Berens, P. H.; Wilson, K. R. A. Computer Simulation Method for the Calculation of Equilibrium Constants for the Formation of Physical Clusters of Molecules: Application to Small Water Clusters. *J. Chem. Phys.* **1982**, *76*, 637−649), a standard algorithm for propagating coordinates, and velocities of particles in molecular dynamics programs. The central image is a rendering of a star polymer, which is a polymeric material topologically consisting of several arms chemically bonded to a common molecular framework (core). Each of the sixteen arms on this particular star polymer is a diblock copolymer with a polyester-based hydrophobic region close to the core and a polyethylene glycol (PEG)-based hydrophilic region (blue) farther away (see: Swope, W. C.; Carr, A. C.; Parker, A. J.; Sly, J.; Miller, R. D.; Rice, J. E. Molecular Dynamics Simulations of Star Polymeric Molecules with Diblock Arms, a Comparative Study. *J. Chem. Theory Comput.* **2012**, *8*, 3733−3749). The conformation shown on the cover is from an all atom molecular dynamics simulation of the polymer in explicit water, with the water molecules not shown. In an aqueous environment, the hydrophobic material collapses into a dense layer around the core and the hydrophilic material remains well-solvated. These molecular architectures have been proposed as potential vehicles for the delivery of hydrophobic drug molecules (see Appel, E. A.; Lee, V. Y.; Nguyen, T. T.; McNeil, M.; Nederberg, F.; Hedrick, J. L.; Swope, W. C.; Rice, J. E.; Miller, R. D.; Sly, J. Toward Biodegradable Nanogel Star Polymers via Organocatalytic ROP. *Chem. Commun.* **2012**, *48*, 6163−6165). Near the top is a molecule of ibuprofen, a representative hydrophobic molecule, adsorbed on the star polymer at the water-hydrophobic material interface. This rendering of the van der Waals surface was produced using the VMD (Humphrey, W.; Dalke, A.; Schulten, K. VMD - Visual Molecular Dynamics, *J. Mol. Graphics*, **1996**, *14*, 33−38. http://www.ks.uiuc.edu/Research/vmd/) molecular graphics program. Around the edges of the cover image are representative conformations that result from coarse-grained simulations of the synthetic process of polymer formation. The image conveys the temporal order in which regions of the polymer formed, with red indicating material that bonded early and blue indicating material that bonded late during the synthetic process. The white spheres represent functional groups in the polymer, places for further reaction, or potential cargo binding. This part of the figure was also produced using the VMD molecular graphics program. We wish to thank Dr. Amber Carr and Nadine Head-Gordon for effort and ideas related to the cover artwork. This special issue was organized by Guest Editors Teresa Head-Gordon and Julia Rice.

SPECIAL SECTION: WILLIAM C. SWOPE FESTSCHRIFT

Guest Editors: Teresa Head-Gordon and Julia Rice

Special Issue Preface

Articles

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