DY 17: Theory and Simulation (joint session CPP/DY)

Time: Friday 13:30–15:00   Location: H3

Invited Talk   DY 17.1   Fri 13:30   H3
Data-driven protein design and simulation — •Andrew Fer-guson — University of Chicago, Chicago, IL, USA

Data-driven modeling and deep learning present powerful tools that are opening up new paradigms and opportunities in the understanding, discovery, and design of soft and biological materials. In this talk, I will first describe an approach integrating ideas from dynamical systems theory, nonlinear manifold learning, and deep learning to reconstruct protein folding funnels and molecular structures from one-dimensional time series in experimentally measurable observables obtainable by single molecule FRET. I will then describe our recent development and application of deep representational learning to expose the sequence-function relationship within homologous protein families and to use these principles for data-driven design of synthetic proteins with new and/or elevated function.

DY 17.2   Fri 14:00   H3
Are there knots in chromatin? — •Peter Virnau — Institut für Physik, Staudingerweg 9, Johannes Gutenberg-Universität Mainz, 55128 Mainz

The rise of HiC chromosome capture methods has recently enabled low-resolution structures of interphase chromatin [1]. In this presentation I will explain how structures based on single cell contact matrices are obtained from simulations of coarse-grained bead-spring polymer Go models [2]. The role of self-entanglements which naturally occur in this process [2,3] will be critically assessed in the light of theoretical arguments and recent experiments [4].
[1] T.J. Stevens et al, Nature 544, 59-64 (2017). [2] S. Wettermann et al, Comp. Mat. Sci 173, 109178 (2020). [3] J.T. Siebert et al, Polymers 9, 317 (2017). [4] D. Goundaroulis, Biophys. J. 118, 2268-2279 (2020).

DY 17.3   Fri 14:15   H3
Surface Segregation in Athermal Polymer Blends due to Conformational Asymmetry — •Russell Spencer[1] and Mark Matsen[2] — [1]Georg-August Universität Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany — [2]University of Waterloo, Waterloo, Ontario, Canada

Monte Carlo simulations are used to investigate the surfaces of athermal blends of stiff and flexible polymers. We vary the bending modulus of the stiff polymers, κ, from zero to the point where the bulk undergoes an isotropic-to-nematic transition. For hard walls characteristic of polymer/solid surfaces, the flexible polymers generally segregate to the surface. However, prior to the bulk transition, there is a surface ordering transition, where a thin nematic layer rich in stiff polymers forms at the surface. On increasing κ further, the thickness of the nematic layer rapidly increases as the bulk isotropic-to-nematic transition is approached. For soft boundaries representative of polymer/air surfaces, a thin layer rich in stiff polymers but without nematic order forms on the outer edge of the surface with a more significant layer rich in the flexible chains beneath. In this case, the nematic layer never appears, and the surface profile evolves continuously with increasing

κ.

DY 17.4   Fri 14:30   H3
Ultra-coarse-graining of homopolymers in inhomogeneous systems — •Fabian Berressem[1], Christoph Scherer[2], Denis Andrienko[2], and Arash Nikoubashman[1] — [1]Johannes Gutenberg University, Mainz — [2]Max Planck Institute for Polymer Research, Mainz

We develop coarse-grained (CG) models for simulating homopolymers in inhomogeneous systems, focusing on polymer films and droplets. If the CG polymers interact solely through two-body potentials, then the films and droplets either dissolve or collapse into small aggregates, depending on whether the effective polymer-polymer interactions have been determined from reference simulations in the bulk or at infinite dilution. To address this shortcoming, we include higher order interactions either through an additional three-body potential or a local density-dependent potential (LDP). We parameterize the two- and three-body potentials via force matching, and the LDP through relative entropy minimization. While the CG models with three-body interactions fail at reproducing stable polymer films and droplets, CG simulations with an LDP are able to do so. Minor quantitative differences between the reference and the CG simulations, namely a slight broadening of interfaces accompanied by a smaller surface tension in the CG simulations, can be attributed to the deformation of polymers near the interfaces, which cannot be resolved in the CG representation, where the polymers are mapped to spherical beads.

DY 17.5   Fri 14:45   H3
How to accurately estimate the specific heat of liquid polymers? — •Debashish Mukherji[1], Hongyu Gao[2], Tobias P. W. Menzel[2], and Martin H. Mueser[2] — [1]Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada — [2]Department of Materials Science and Engineering, Saarland University, 66123 Saarbruecken, Germany

The field of atomistic simulations of polymers is in a mature stage, yet predictions of specific heat from molecular simulations and successful comparisons with experimental data are scarce if existing at all. One reason for this may be that the internal energy and thus the specific heat cannot be coarse-grained so that they defy their rigorous computation with united-atom models. Moreover, many modes in a polymer barely contribute to the specific heat because of their quantum mechanical nature. Here, we adopt an existing method [1], which defines a specific heat for a harmonic reference, to estimate the specific heat difference between classical and quantum-mechanical systems and use this as a correction factor. Thereby, we predominantly correct the stiff, high-frequency harmonic modes, while leaving the specific-heat contributions of the slow (anharmonic) modes intact [2]. We show how to construct corrections for both all-atom and united-atom descriptions of chain molecules. Corrections computed for a set of hydrocarbon oligomers and commodity polymers deviate by less than kB/10 per particle. The results compare well with experimental data.
[1] Horbach, Kob, and Binder, JPCB 103, 4104 (1999). [2] Gao, Menzel, Mueser, and Mukherji, PRM 5, 065605 (2021).