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Atomic-level simulations of biomolecular systems with a modified Amber force field

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Experimental methods have been highly successful in determining 3-dimensional biomolecular structures. However, most approaches provide only time- or ensemble-averaged data, making it much more difficult to study the dynamic and energetic aspects of biological systems. Atomic-resolution simulations are highly complementary to experiments, and can provide data with unparalleled resolution in time and space. Due to the long timescales of biologically relevant events, as well as the complexity of the energy function, accurate and precise simulations remain highly computationally challenging. This seminar will highlight recent progress in both areas, illustrating how energy functions that have been trained on simple peptide models can be successfully used for the study of much more complex systems. We demonstrate that our newly trained energy parameters significantly reduce the secondary structure bias reported for previous Amber parameter sets. Applications of the parameters include studies of folding behavior of peptides and small proteins, and the dynamic behavior of larger biomolecular systems such as conformational changes during drug binding in HIV-1 protease.