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Biophysical Discovery through the Lens of a Computational Microscope

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With exascale computing power on the horizon, improvements in the underlying algorithms and available structural experimental data are enabling new paradigms for chemical discovery. My work has provided key insights for the systematic incorporation of structural information resulting from state-of-the-art biophysical simulations into protocols for inhibitor and drug discovery. We have shown that many disease targets have druggable pockets that are otherwise "hidden" in high resolution x-ray structures, and that this is a common theme across a wide range of targets in different disease areas. We continue to push the limits of computational biophysical modeling by expanding the time and length scales accessible to molecular simulation. My sights are set on, ultimately, the development of detailed physical models of cells, as the fundamental unit of life, and two recent achievements highlight our efforts in this arena. First is the development of a molecular and Brownian dynamics multi-scale modeling framework, which allows us to investigate drug binding kinetics in addition to thermodynamics. In parallel, we have made significant progress developing new tools to extend molecular structure to cellular environments. Collectively, these achievements are enabling the investigation of the chemical and biophysical nature of cells at unprecedented scales.