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Editorial

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Special Issue on Free Energy

Free energy has been recognized as a central concept in the physical sciences since the early 19th century. In the ensuing decades, the importance of changes in free energy in governing chemical equilibria and—with dynamical corrections—in determining rates of chemical processes has become universally appreciated. Accordingly, there has been an unending drive to develop more accurate and facile methods to calculate free energy changes and to apply these to the study of molecular recognition and binding, the kinetics of molecular transformations, and myriad other processes. In the past 30 years or so, advances in theoretical chemistry and computational resources have enabled free energy calculations to emerge as a useful tool in studies of conformational changes, the physical process of complex formation, and chemical reactions. Unique to theoretical studies, "computational alchemy" was invented to allow, e.g., the transformation of one candidate drug into another, both within a binding site and in solution; thermodynamic cycle arguments allow the correspondingly computed free energy differences to be used to predict the experimental difference in free energy of binding of the two drugs. Despite this progress, practical challenges still remain in ensuring the accuracy of the potential functions used in such calculations and in the adequate sampling of configurations of the systems studied. To assess the current state of this field and identify possible paths forward, the workshop "Free Energy Calculations: Three Decades of Adventure in Chemistry and Biophysics" was held in Snowmass, Colorado, in July 2013. Participants in this lively meeting were invited to contribute manuscripts for this special issue of *JCTC*. The special issue builds on the discussions at the 2013 workshop with many new results, as seen in the following pages.

J. Andrew McCammon,* co-organizer
University of California at San Diego, San Diego, California, United States
Benoit Roux, co-organizer
University of Chicago, Chicago, Illinois, United States
Gregory Voth, co-organizer
University of Chicago, Chicago, Illinois, United States
Wei Yang, co-organizer
Florida State University, Tallahassee, Florida, United States

AUTHOR INFORMATION

Corresponding Author
*E-mail: jmccammon@mail.ucsd.edu.

Notes
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Special Issue: Free Energy Calculations: Three Decades of Adventure in Chemistry and Biophysics

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