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Free-energy calculations in soft and hard matter: From Hamiltonian thermodynamic integration to early applications of umbrella sampling

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Free energy is a thermodynamic potential that plays a pivotal role in comprehending the behavior of energy processes and transformations in matter. However, the development of accurate methods to calculate it has been a significant challenge for scientists involved in analytical and computer simulation approaches, spanning several generations. This presentation seeks to provide an analysis of the most significant works related to free-energy calculations, along with a chronology and primary-source collection that is valuable for gaining historical insights. The period under review commences with the analytical studies of John Kirkwood in 1935, which laid the foundations for the Hamiltonian thermodynamic integration, and extends to the emergence of umbrella sampling in 1977. The focus will be on simulative techniques and the major challenges that molecular simulation practitioners faced. Despite some references in natural-science literature, a systematic documentation of the history of free-energy calculations is lacking. Hence, this talk aims at presenting the initial few strides made in this direction.

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