Special Issue

Free Energy and Entropy Changes: From Molecular Dynamics Simulations to the Developing Theories of Small Systems

Message from the Guest Editors

This Special Issue serves as a platform for presentation of results in the wide context of non-equilibrium systems, with specific focus on new and improved techniques developed for estimation of free energy changes in macromolecular systems, or more in general on the study of the fluctuations of thermodynamics quantities such as heat, work or entropy production in different systems. Original research papers, reviews/perspectives and short communications covering theory and applications are welcome.

- ensembles
- free energy
- work
- mesoscopic systems
- foundations
- protein stretching
- stochastic thermodynamics
- absolute irreversibility
- virial
- non-equilibrium

Guest Editors

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Deadline for manuscript submissions

closed (31 May 2022)



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Impact Factor 2.0
CiteScore 5.2
Indexed in PubMed



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Message from the Editor-in-Chief

The concept of entropy is traditionally a quantity in physics that has to do with temperature. However, it is now clear that entropy is deeply related to information theory and the process of inference. As such, entropic techniques have found broad application in the sciences.

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