



entropy



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Configurational Entropy

Guest Editor:

Dr. Vladimir Hnizdo

National Institute for
Occupational Safety and Health,
Morgantown, WV 26505, USA

Deadline for manuscript
submissions:

closed (30 April 2010)

Message from the Guest Editor

Dear Colleagues,

Changes in the configurational part of entropy contribute significantly to the free energy of conformational change and binding in biomolecular systems. In particular, the change in configurational entropy is an important determinant of the energetics of the binding affinity in receptor-ligand systems. However, calculating the configurational entropy of complex non-harmonic systems is a highly challenging problem in need of innovative approaches to a practicable solution. Recently, information-theoretic methods and nonparametric statistical methods have been brought to bear on the problem of estimating configurational entropy from molecular simulations. This special issue of Entropy will provide a forum for contributions on both theoretical and computational aspects of the entropic characteristics of complex systems.

Dr. Vladimir Hnizdo

Guest Editor



mdpi.com/si/82

Special Issue



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Editor-in-Chief

Prof. Dr. Kevin H. Knuth

Department of Physics, University
at Albany, 1400 Washington
Avenue, Albany, NY 12222, USA

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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Entropy Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

Tel: +41 61 683 77 34
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