Special Issue

The Information-Theoretic Approach in Density Functional Theory and Beyond

Message from the Guest Editor

This Special Issue aims to be a forum for the presentation of different methodologies, techniques, and applications of ITAs in DFT and other theoretical frameworks to problems for molecular and other systems. It is the humble view of the present that ITA quantities, as simple yet explicit density functionals, provide much more information about physicochemical properties of molecular and other electronic systems and should deserve our close attention when we develop a reactivity theory in DFT language and/or another electronic structure theory in quantum chemistry.

Guest Editor

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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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Editor-in-Chief

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