Special Issue

Computational Physics and Chemistry Contributions to the Investigation of Ionic Liquids

Message from the Guest Editors

Ionic liquids have largely been investigated for their peculiar experimental properties and their uncountable applications. From a computational point of view, they pose many challenges, mainly because they are composed of ions, and at ambient temperature and pressure most of them take liquid form, lacking a periodic structure. Describing mixtures of ionic liquids with other ionic liquids or molecular solvents is an even greater challenge. Computational chemistry and physics provide important contributions for understanding the reported properties of ionic liquids and mixtures, rationalizing them and predicting behaviors that have yet to be experimentally investigated. We invite contributions to this Special Issue concerning new computational contributions to explain or rationalize ionic liquids' properties and their use in real applications.

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Deadline for manuscript submissions

closed (31 July 2023)

Entropy

an Open Access Journal by MDPI

Impact Factor 2.0
CiteScore 5.2
Indexed in PubMed

mdpi.com/si/106651

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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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