Special Issue

Halogen Bonding: Insights from Computational Tools

Message from the Guest Editor

The distinctive features of halogen bonds have prompted their widespread application in many areas such as supramolecular chemistry, crystal engineering, catalysis, medicinal chemistry, and chemical biology, among others. Given their relevance, computational and molecular modeling methods are extremely helpful in the quest for further understanding the phenomenon or to guide new experimental work. Indeed, theoretical studies are in the frontline of quarrels concerning the nature of the halogen bond, and the study of solvent and substituent effects. This Special Issue aims to highlight the role of computational methodologies in the study of halogen bonds, ranging from the most common quantum mechanics calculations to force field-based methods. Therefore, original manuscripts reporting the application of computational tools in the study of halogen-bonded systems are encouraged. In addition, perspectives and reviews are also welcome.

Guest Editor

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Deadline for manuscript submissions

closed (15 February 2020)

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/si/21009

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As the premier open access journal dedicated to molecular chemistry, now in its 29th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts, and novel materials. Pushing the boundaries of the discipline, we invite papers on all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

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