Special Issue

Open-Shell Systems for Functional Materials

Message from the Guest Editors

Open-shell systems are widely noticed from the viewpoint of fundamental studies on their peculiar characteristics, applications to materials and an understanding of the biological functions. Theoretical calculations are now one of the powerful tools for understanding such systems. However, these systems are, in a sense, still challenging subjects because they are usually large and orbitally-degenerated systems with localized electron spins (localized orbitals). In this Special Issue, we focus on recent developments, advances and future prospects of open-shell systems. We welcome contributions from both experimental and theoretical researchers, as well as cooperative studies between theories and experiments. Topics to be discussed cover a broad range of fields concerning open-shell systems, from basic theory in quantum theory, fundamental material science, applications in functional materials and biosystems, etc. We also welcome the intersectional area between material science and biomolecular science.

Guest Editors

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Deadline for manuscript submissions

closed (31 December 2018)



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Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th 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 multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

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