Journal of Chemistry

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Special Issue on

Novel Materials with Photochemical, Photocatalytic, and Photophysical Properties: Theoretical Approaches

CALL FOR PAPERS

Unique electronic and chemical properties of nature, coming from light-matter interactions, have drawn the attention of researchers who wish to understand them with the aim of developing new generation devices. The most prominent example triggering important chemical reactions for life is photosynthesis, where the light harvesting, charge separation, and catalysis are combined together to carry out the thermodynamically demanding processes such as oxidation of water and the reduction of carbon dioxide.

The photochemical, photophysical, and photocatalytic processes are at the heart of important emerging technologies such as 3D optical memories based on photoswitching molecular materials in the new generation of solar cells. In this context, photoelectrochemical biosensors developed from these types of solar cells have received increasing attention due to their desirable sensitivity and better analytical performance. On the other hand, the low-frequency irradiation to metal nanoparticles leading to heat generation is currently used in photothermal therapies for cancer treatment. For these reasons and many more ones, a deep understanding of the photochemical, photocatalytic, and photophysical processes at the molecular level is a relevant problem of chemical science.

Theoretical calculations have been proven to be useful to gain insight into the mechanisms directly related to the absorption/emission phenomena of molecules. Among the available approaches for the study of optical properties of even large systems that are still being developed are DFT, linear scaling TD-DFT, tight-binding DFT, and semiempirical and hybrid procedures such as Quantum Mechanics/Molecular Mechanics. In recent years, the exponential increase in computing power has allowed the access to higher level calculations for some reduced systems by post-Hartree-Fock approaches, such as Møller–Plesset (MP2), complete active space second-order perturbation theory (CASPT2), and Coupled Cluster Singles and Doubles (CCSD).

This special issue will focus on the theoretical evaluation of electronic properties of materials with appealing photochemical, photocatalytic, and photophysical properties with use in a wide range of applications. We encourage submissions on the theoretical study of new systems properties with application in various fields.

Potential topics include but are not limited to the following:

- Optical properties of solid materials
- Light energy conversion in materials with photovoltaic applications
- Solar cells as photovoltaic materials
- Photophysical characterization of new chromophores
- Photophysical properties of biomarkers and biosensors
- Photochemical mechanisms of generation of reactive oxygen species
- Photochemistry of supramolecular systems and nanostructures
- Modelling of two-photon absorption processes
- Theoretical and computational methods applied to photochemical systems

Authors can submit their manuscripts through the Manuscript Tracking System at https://mts.hindawi.com/submit/journals/jchem/theoretical.chemistry/nmpp/.

Papers are published upon acceptance, regardless of the Special Issue publication date.

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