

Special Issue on
Theoretical Modeling of the Optical Properties of 2D Materials

CALL FOR PAPERS

Two-dimensional materials, constituted by single- or few-layer sheets of atoms, have emerged in the last ten years, soon after the discovery of graphene, as a source of continuously growing potential applications. On one side, the effort of mimicking the exceptional properties of graphene has been pursued by investigating the possible realizability of nanosheets based on single-element group-IV atoms, such as silicene, germanene, and stanene. On the other side, borrowing from graphene the idea of a 2D material obtained by exfoliation, other layered materials are extensively investigated, such as h-BN, transition metal dichalcogenides (MoS_2 , WS_2 , MoSe_2 , WSe_2 , MoTe_2 , WTe_2 , ZrS_2 , ZrSe_2 , NbSe_2 , NbS_2 , TiSe_2 , NiSe_2 , GaSe , GaTe , InSe , Bi_2Te_3 , and Bi_2Se_2), black phosphorus, h-BNC, fluorographene, graphene oxide, 2D silica, and 2D Pb. In addition, hybrid structures as well as the heterostructures of the materials mentioned above can be imagined and designed.

Among the several intriguing and progressively explored peculiarities of such nanosheets, optical properties play a very significant role for the possibility of tailoring amplitude and nature of the band gap (e.g., by controlling the number of layers, by engineering heterostructures, by strain, or by electric field or magnetic field (magnetic impurities)) and for the very large effect that quantum confinement and reduced screening have in 2D systems. This provides the conceptual basis of innovative devices for generating or detecting light with a wealth of potential applications in photonics, optoelectronics, energy harvesting, quantum anomalous Hall effect (QAHE), quantum spin Hall effect (QSHE), and so forth. Theoretical modeling is an essential step to accurately investigate the properties of materials that are often first predicted by theory and then realized experimentally.

The purpose of this special issue is to publish high-quality research papers as well as review articles addressing recent advances on theoretical modeling and computational methods for the study of the optical properties of two-dimensional materials. Original, high-quality contributions that are not yet published and that are not currently under review by other journals or peer-reviewed conferences are welcome.

Potential topics include but are not limited to the following:

- ▶ Nanosheets based on group-IV elements
- ▶ Layered materials
- ▶ Heterostructures
- ▶ 2D crystals on substrates
- ▶ Optical modulators and optical sensors based on 2D materials
- ▶ 2D materials optics such as nonlinear optics, photonics, and electro- and photochromics
- ▶ 2D materials based display technologies such as LEDs and OLEDs and liquid crystals
- ▶ Computational screening of 2D materials for photocatalysis
- ▶ 2D materials for high-performance energy storage applications
- ▶ Theoretical approaches and computational methods: random phase approximation, time-dependent density functional theory, many-body perturbation theory, and tight binding

Authors can submit their manuscripts through the Manuscript Tracking System at <http://mts.hindawi.com/submit/journals/acmp/tmop/>.

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