

2D materials

Cite as: J. Chem. Phys. **154**, 040401 (2021); <https://doi.org/10.1063/5.0043003>

Submitted: 05 January 2021 • Accepted: 06 January 2021 • Published Online: 29 January 2021

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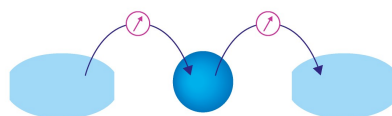
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Submitted: 5 January 2021 • Accepted: 6 January 2021 •

Published Online: 29 January 2021



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Note: This paper is part of the JCP Special Topic on 2D Materials.

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<https://doi.org/10.1063/5.0043003>

Two-dimensional (2D) systems have long been the domain of important studies in chemical physics. The field of 2D materials profoundly changed with the advent of the isolation and investigation of graphene. While graphene continues to dazzle the research community with recent discoveries such as superconductivity and highly correlated electron physics in twisted bilayers, a plethora of other 2D materials has emerged, covering an entire spectrum of electronic and optical properties. The possibility of stacking these 2D materials to create designer structures has opened the door to unprecedented control of the properties of these ultrathin systems. Our focus issue on 2D materials highlights key fundamental questions that have been opened by the creation of these materials, such as excitonic behavior, charge and energy transfer, and quantum confinement in electronic and phononic degrees of freedom.

Graphene, the best-known 2D material, continues to surprise us. In an exciting development, Li *et al.* showed that the optical non-linearity of graphene can readily be controlled by electrostatic gating.¹ The authors attributed this finding to the unique band structure of graphene, which allows for quantum interference among multiple nonlinear transition pathways. Kim and Cui applied graphene as a temperature sensor and demonstrated a markedly increased sensitivity when graphene is suspended over holes created in anodic aluminum oxide.² Gravelle *et al.* provided a detailed simulation of the process of liquid exfoliation of graphene using molecular dynamics.³

In 2D semiconducting transition metal dichalcogenides (TMDCs), trions, three-body charged bound states, have attracted the attention of a number of authors. Zipfel *et al.* investigated trion dynamics in WS₂ monolayers and showed the important role of exchange splitting in determining their non-equilibrium energy distribution and slow cooling rate.⁴ Goldstein *et al.* probed excitons as a function of carrier doping in MoSe₂. These authors suggested that the exciton–polaron model provides a better description of experimental results than the few-body trion model does.⁵

In contrast, theoretical analysis by Glazov suggested that the few-body quasiparticle description and the many-body Fermi–polaron treatment produce equivalent results for trions in atomically thin 2D semiconductors in the low doping limit.⁶ Zhumagulov *et al.* carried out a theoretical analysis of trions in a doped MoS₂ monolayer and suggested that non-zero momentum transitions can explain their photoluminescence line shape and temperature dependence.⁷ Carbone *et al.* developed a fully microscopic model for the doping-dependent exciton and trion linewidths in TMDC monolayers in the low-doping limit.⁸ These authors revealed that the trion linewidth is relatively insensitive to doping levels, while the exciton linewidth increases monotonically with doping, in agreement with experiments.

Theory has also been essential in guiding the research on other 2D materials. Philbin *et al.* carried out a theoretical analysis of Auger recombination for bi-exciton decay in nanoplatelets and showed the general scaling of this process with the area and thickness.⁹ Agrawal *et al.* carried out an *ab initio* quantum dynamics study of charge carriers in graphitic carbon nitride nanosheets that are of interest in photovoltaic and photocatalytic applications.¹⁰ Patra *et al.* reported new methodology development associated with nonuniform density scaling in quasi-two-dimensions.¹¹

2D layered perovskites represent a class of versatile optoelectronic materials. Dahod *et al.* analyzed phonon spectra of 2D layered perovskites by low-frequency Raman spectroscopy. In addition to optical phonon modes, these authors revealed longitudinal acoustic phonons corresponding to the motion of the layered superlattice structure.¹² Do *et al.* carried out photoluminescence spectroscopy studies of 2D layered perovskites and revealed the presence of both momentum direct and indirect excitons.¹³

Developing reliable methods to probe atomically thin 2D materials is essential for structural characterization. One of the most overlooked problems in the study of 2D materials is the omnipresence of strain and mechanical deformation in the samples. Darlington

et al. presented a facile method for strain analysis in nanobubbles in 2D semiconductors, confirming the analysis by hyperspectral nano-optical imaging.¹⁴ On a freestanding 2D material, one expects a high level of contaminants from molecular adsorption and/or polymer residuals in handling. Using ion spectroscopy, Niggas *et al.* showed the extensive presence of contaminants, which may be reduced by thermal annealing.¹⁵

Defects in 2D materials often present high chemical reactivities. Gao *et al.* addressed the application of graphene in electrocatalysis, which occurs predominantly at the edges that can be increased by creating holes in graphene electrodes.¹⁶ Peng *et al.* showed that oxygen doping in MoS₂ quantum dots increases the efficiency of electrocatalytic hydrogen generation.¹⁷ Stesmans *et al.* analyzed variations in paramagnetic defects and dopants in MoS₂ from diverse geosources.¹⁸

One aspect of the versatility of 2D materials is the ability to create heterojunctions in an easy manner. Wang *et al.* used first principles calculations to investigate metal–bilayer MoS₂ junctions.¹⁹ These authors reported multiple mechanisms for charge redistribution at the metal–semiconductor junction. He *et al.* carried out electronic structure calculations of the Ti₂O/WTe₂ van der Waals heterostructure.²⁰ These authors showed that a straddling type-I band alignment can be transformed into a staggered type-II alignment via strain or electric field. Canton-Vitoria *et al.* experimentally demonstrated the stabilization of metallic phases of monolayer MoS₂ through lateral heterostructures with the semiconducting phase of MoS₂ and suggested that the same approach may be applied to other TMDC monolayers.²¹

Several papers reported new structures and phases of 2D materials. Baskurt *et al.* reported 1T- and 1H-phases of single layers of calcium halides.²² Akahama *et al.* determined the structural motifs of black phosphorus under high pressure.²³ Ziogos *et al.* reported new 2D molecular semiconductors with bandgaps in the visible range from porphyrin and tetra-indole covalent organic frameworks.²⁴ Yoshinobu *et al.* reported the formation of BN-covered silicene from surface chemical reactions.²⁵

These papers provide a selective sampling of the growing field of 2D materials. The collection provides a wide vista from which one can understand the uniqueness of these systems from extreme quantum confinement, from van der Waals interfaces and heterojunctions, and from the rich variations in electronic coupling, local symmetry, and chemical reactivity.

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