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## GUEST EDITORIAL

# Chemical Functionalization of 2D Materials

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This special issue on the “Chemical Functionalization of 2D Materials” is a celebration of cutting-edge advances in the field of 2D materials, showcasing a curated collection of outstanding contributions from leading experts in the field and the next generation of innovators.

Originally conceived to complement Symposium J, “Chemical Functionalization of 2D Materials,” at the 2024 European Materials Research Society (E-MRS) Spring Meeting held in Strasbourg, France, this issue captures the spirit of innovation and collaboration that defines the global 2D materials community. Through these articles, we aim to highlight both foundational progress and forward-looking perspectives that continue to drive the field toward exciting new frontiers.

This Editorial offers a dynamic overview of the diverse world of 2D materials, exploring their unique structures and the transformative potential of chemical functionalization. From tailoring electronic and optical properties to unlocking entirely new functionalities, we delve into how strategic chemical modifications can elevate the performance of 2D materials across a wide range of cutting-edge applications. These curated insights set the stage for the exciting developments presented throughout this special issue.

2D materials—atomically thin layers with exceptional physical, chemical, and mechanical properties—have transformed the landscape of materials science since the discovery of graphene. Defined by their high surface-to-volume ratios, tunable band

structures, and remarkable carrier mobility, 2D materials serve as a dynamic platform for innovations across areas such as electronics, photonics, energy, and biotechnology. The family of 2D materials has rapidly expanded beyond graphene to include transition metal dichalcogenides (TMDs), MXenes, black phosphorus, boron nitride, and metal organic framework (MOF) nanosheets, each offering distinct functionalities.

With their ultrathin, flexible nature, these materials are highly responsive to surface modifications, making them ideal candidates for chemical functionalization. This approach enables precise tuning of interfacial chemistry, structural stability, and physicochemical properties, pushing the boundaries of performance in complex environments. As research advances, functionalization is poised to play a pivotal role in translating the unique capabilities of 2D materials into real-world technologies.

The chemical functionalization of 2D materials has emerged as a powerful and fast-expanding frontier in materials science, offering unprecedented opportunities to tailor and enhance their intrinsic properties. By introducing functional groups or molecular moieties onto 2D surfaces, researchers can not only prevent undesirable aggregation in solvents, thereby preserving high aspect ratios and surface areas, but also significantly improve dispersibility, wettability, and processability. More importantly, this approach opens the door to precisely tuning the electronic, optical, chemical, and mechanical properties of 2D materials, as well as unlocking entirely new behaviors not observed in their pristine forms.

These chemically engineered 2D materials have demonstrated immense promise across a broad spectrum of applications, including next-generation energy storage and conversion systems, multifunctional nanocomposites, flexible electronics, catalysis, and high-sensitivity sensors. For instance, functionalized graphene can form robust interfacial bonds with polymers, yielding nanocomposites with dramatically improved mechanical strength and durability. Similarly, surface-modified TMDs have been leveraged to fine-tune charge transport and catalytic activity, making them attractive for use in transistors, electrocatalysts, and photodetectors.

Several important review articles featured in this issue provide a comprehensive and timely overview of these developments, reflecting the growing maturity and impact of the 2D materials field. Guo, Jia, He, and co-workers introduce 2D material/self-assembled monolayer (SAM) heterostructures as a powerful platform for tuning interfacial properties, enabling enhanced performance and versatility in next-generation electronic devices (2402857). Complementing this, Yan and his team explore substrate engineering strategies, such as strain modulation and charge doping, to elevate the chemical reactivity of graphene by manipulating its interaction with supporting materials (2408116). On the preparation front, Zhang and colleagues provide critical insights into the controlled fabrication of noble TMDs via thermally assisted conversion and chemical vapor deposition, underscoring their promise in electronics, optoelectronics, and electrocatalytic systems (2407233). Meanwhile, Cheng, Wu, and collaborators delve into the realm of energy storage, offering a detailed account of advanced fabrication techniques and charge-storage mechanisms in TMD-based cathodes for aqueous zinc-ion batteries, with an emphasis on structural innovation and performance optimization (2410036).

Collectively, these review articles not only summarize the state-of-the-art progress but also chart future directions, highlighting the transformative potential of 2D materials across multiple technological domains.

This special issue also features a vibrant collection of original research articles showcasing the remarkable versatility and continued evolution of 2D materials across multiple domains, including electronics, sensing, energy conversion and storage, catalysis, and photonics. The contributions demonstrate innovative material design, interface engineering, and device integration strategies that unlock new levels of functionality and performance.

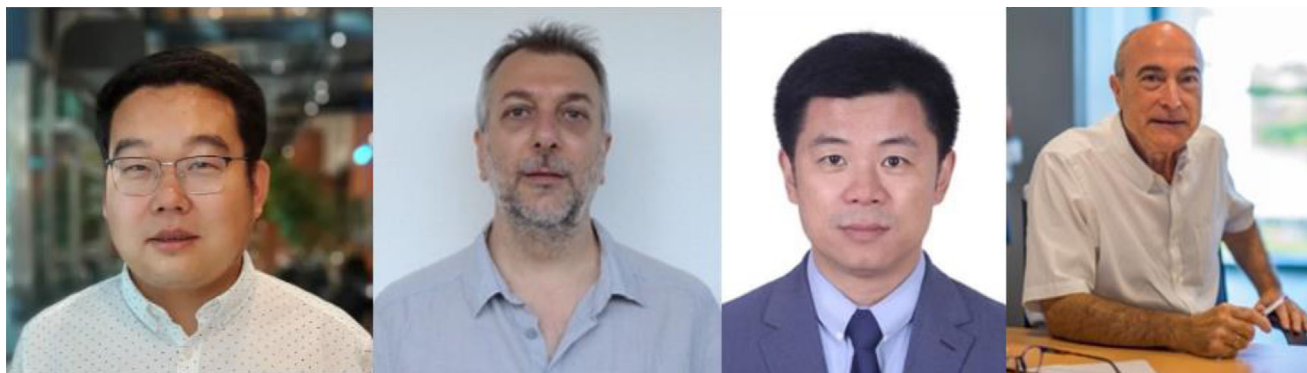
**Electronic Devices and Sensing:** Innovative electronic devices and sensors built from functionalized 2D materials are spotlighted. Zhang and co-workers stabilized black phosphorus nanosheets through viologen-based noncovalent functionalization, preserving their ambient integrity for energy and optoelectronic applications (2410300). Samori and colleagues developed a light-tunable humidity sensor based on spiropyran-functionalized MoS<sub>2</sub> transistors, where reversible photoisomerization modulates charge transport and wettability under different humidity conditions (2404633). Hou, Zhang, and co-authors engineered a dodecylamine-functionalized GO Fabry–Perot acoustic sensor with ultra-high sensitivity in the 10–200 Hz range and a minimum detectable pressure of 0.333  $\mu\text{Pa Hz}^{-1/2}$  (2409043). Schneider, Fu,

and collaborators designed a pyrene-anchored, substrate-tight graphene transmembrane nanofluidic platform that prevents delamination, boosting device success rates from ~4% to ~76% – critical for robust nanopore technologies (2407140).

**Energy Storage and Conversion:** Several works explore advanced 2D materials tailored for high-efficiency energy storage. Rui, Yu, and co-workers developed a solid-state self-assembly strategy to construct Na<sub>3</sub>V<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub>@carbon spherical superstructures, achieving outstanding sodium-ion storage and excellent low-temperature performance down to –40 °C (2407285). Shin, Dunn, Park, and colleagues introduced BN@rGO nanosheets for dual-ion and zinc-alkaline full cells, enabling a high voltage window (~1.7 V), robust capacity (~58 mAh g<sup>-1</sup>), and exceptional cyclability (2405548). Meanwhile, Li and his team proposed a lithium pre-intercalation approach in  $\lambda$ -Li<sub>x</sub>MnO<sub>2</sub> for selective Li<sup>+</sup> recovery from low-grade brines, offering high capacity (~33.7 mg g<sup>-1</sup>), excellent selectivity (factor  $\approx$  32.7), and low energy consumption (2406951). In the realm of anode-free batteries, Wang, Wagemaker, and Bannenberg devised a tailored electrolyte formulation featuring Li-salt and propylene carbonate, which enabled the formation of a ZnF<sub>2</sub>-rich solid electrolyte interphase on MXene current collectors, dramatically improving Zn deposition uniformity and achieving a Coulombic efficiency of up to 96.8% over 150 cycles (2407226). Zhang, Yang, and co-workers further advanced LIB anode development by Co-doping Fe<sub>2</sub>N@C nanosheets, tuning the work function to enhance charge transfer and Li<sup>+</sup> adsorption, achieving 673 mAh g<sup>-1</sup> specific capacity and excellent rate capability (2405608).

**Photocatalysis and Optoelectronics:** In photocatalysis, Chen, Lu, Jiao, and co-workers introduced a 3D/2D graphene/MXene composite leveraging hot/free electron transfer to drive efficient hydrogen evolution without conventional semiconductors (2407863). Yang and collaborators designed CH<sub>3</sub>- and F-functionalized C<sub>60</sub>-based heterostructures for Z-scheme photocatalytic water splitting, significantly boosting charge separation, reducing reaction barriers, and enhancing light absorption, offering a promising route toward efficient hydrogen production (202504146). Forment-Aliaga and Coronado's liquid-phase strategy enabled the asymmetric decoration of 2D MoS<sub>2</sub> with gold nanoparticles, leading to defect-engineered Janus structures with enhanced B-exciton emission, suitable for catalytic and optoelectronic applications (2406599).

**Synthesis and Processing of Functional 2D Materials:** At the materials processing frontier, Singer and his team developed a self-limiting electrospray deposition technique using methylcellulose nanowire binders to uniformly template functional particle coatings (including Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene) on structured substrates, demonstrating application in microsupercapacitors (2405509). Martínez–Martínez et al. successfully converted flexible spin-crossover MOF macrocrystals into nanocrystals using ultrasound, retaining structural integrity and enabling detailed charge-transport studies via Microcrystal Electron Diffraction (2408966). Pérez, Sebastian, and colleagues synthesized chemically linked heterostructures of Pd nanosheets and 2H-MoS<sub>2</sub> using a bifunctional molecular linker, significantly extending optoelectronic activity into the infrared (up to ~1700 nm), beyond what is achievable with traditional van der Waals interfaces (2406030).



**FIGURE 1** | From left to right: Prof. Xiaoyan Zhang, Prof. Nikos Tagmatarchis, Prof. Zhong-Shuai Wu, Prof. Nazario Martin.

As Guest Editors (Figure 1) of this special issue, we are delighted to present a diverse collection of cutting-edge research focused on the chemical functionalization of 2D materials. This curated selection brings together fundamental insights to application-driven advances, featuring valuable perspectives for both seasoned researchers and those newly engaging with 2D materials.

Collectively, these contributions highlight the expanding capabilities of 2D materials and their hybrids in addressing pressing challenges in energy, electronics, sensing, and catalysis. The diverse strategies explored—from molecular engineering and interface modulation to scalable synthesis and hybrid structure design—not only demonstrate the field's maturity but also underscore the transformative potential of 2D materials in shaping the next generation of technologies.

We hope this special issue serves as both a timely resource and an enduring source of inspiration for the scientific community.

We are deeply grateful to the brilliant scientists who contributed to this special issue, generously sharing their cutting-edge research and helping to shape a compelling vision of the field's future. Their enthusiasm and dedication made this collection not only possible but truly inspiring. We also extend our sincere appreciation to the broader scientific community, whose pioneering studies—cited throughout this issue—laid the essential groundwork for these advances. Our heartfelt thanks go to the outstanding team at Wiley-VCH, particularly the editorial staff of *Small*, for their enthusiasm, precision, and unwavering support from the moment we proposed this special issue. A special tribute goes to Dr. Lisa Smith, whose editorial expertise, energy, and thoughtful guidance were key to transforming our concept into a vibrant and impactful reality.

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#### **Conflicts of Interest**

The authors declare no conflicts of interest.