Solid-state NMR Investigations of 2D Materials

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Nearly two decades have elapsed since the initial triumph in synthesizing graphene. Since then, the intriguing physical, electrical, chemical, and optical features of two-dimensional materials (2DM) have drawn further attention to related materials. 2DMs are ultrathin nanomaterials with special properties such as high surface-to-volume ratio, surface charge, form, high anisotropy, and chemical functionality that may be adjusted. [1]
Solid-state NMR spectroscopy has become a potent tool for examining the dynamics and atomic-level structure of solid materials. [2] One of NMR's main benefits is its capacity to offer comprehensive details about a material's local atomic structure. This is especially relevant for two-dimensional materials, since they frequently have highly anisotropic structures that can be challenging to define with other methods. In this study, we delved into two categories of 2D materials: transition metal carbides/nitrides (MXenes)[2] and covalent organic frameworks (COFs) [3], employing different solid-state NMR experiments.
The structure of 2D COFs and MXenes was investigated with solid-state NMR MAS spectroscopy detecting ^{1}H, ^{11}B, ^{13}C nuclei by employing techniques like cross polarization (CP), heteronuclear correlation spectroscopy (HETCOR), back-to-back (BABA) and multiple-quantum magic angle spinning (MQMAS) experiments. Fast-spinning ^{1}H MAS NMR spectroscopy could be established as a powerful method to visualize and quantify defect and edge sites in 2D COFs. ^{11}B MAS NMR spectroscopy at variable field strength was applied in order to study the coordination state of surface-exposed ^{11}B nuclei in MXenes.
Overall, solid state NMR is a valuable tool for investigating the structure and properties of 2D materials Furthermore, exploring integrations of solid-state NMR spectroscopy with other analytical methods could yield a broader and more profound comprehension of 2D materials.

References

[1] Reif B., Ashbrook S. E., Emsley L., Hong M., Nature Reviews Methods Primers, 2021, 2.
[2] B. Sun et al., Adv. Mater. 34 (2022) 2108682
[3] N. Lopatik et al., Phys. Chem. Chem. Phys. 25 (2023) 30237-30245

Figures

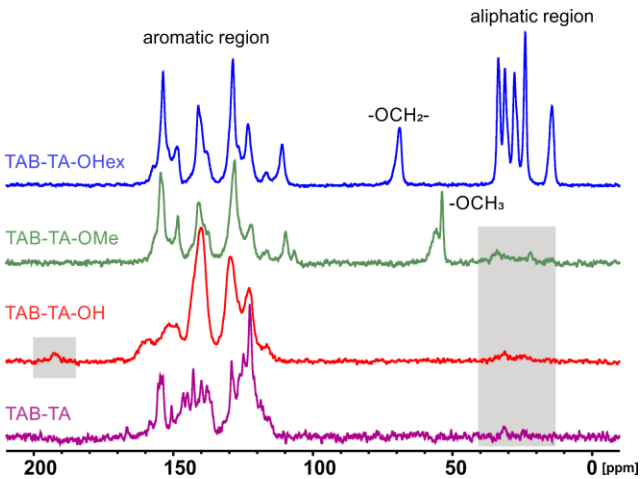

Figure 1: ^{13}C CP MAS NMR spectra of TAB-TA, TAB-TA-OH, TAB-TA-OMe, and TAB-TA-OHex