CHEM2DMAC

Solid-State NMR Investigations of 2D Materials

Nikolaj Lopatik, Ankita De, Dongqi Li, Andreas Schneemann, Minghao Yu, Silvia Paasch, Xinliang Feng, Eike Brunner Technische Universität Dresden, Bergstr. 66, Dresden, Germany nikolaj.lopatik@tu-dresden.de

Almost 20 years have passed since the first successful synthesis of graphene. Since then, related materials have attracted increasing interest due to promising physical, electrical, chemical, and optical properties of two-dimensional materials (2DM). 2DMs are ultrathin nanomaterials and exhibit unique characteristics such as high surface-to-volume ratio, surface charge, shape, high degree of anisotropy and adjustable chemical functionality. ^[1]

Solid-state NMR spectroscopy has emerged as a powerful technique for investigating the atomiclevel structure and dynamics of solid materials. ^[2] One of the key advantages of NMR, its ability to provide detailed information about the local atomic structure of materials, is particularly important for 2D materials, which often have highly anisotropic structures that can be difficult to characterize using other techniques. In this contribution, we investigated two types of 2DMs: transition metal carbides/nitrides (MXenes)^[3] and covalent organic frameworks (COFs), using various solid-state NMR experiments.

The structure of 2D COFs and MXenes was investigated with solid-state NMR MAS spectroscopy detecting ¹H, ¹¹B, ¹³C nuclei by employing techniques like cross polarization (CP), heteronuclear correlation spectroscopy (HETCOR) and the back-to-back (BABA) NMR multiple pulse sequence. Fast-spinning ¹H MAS NMR spectroscopy could be established as a powerful method to visualize and quantify defect and edge sites in 2D COFs.^[4] ¹¹B MAS NMR spectroscopy at variable field strength was applied in order to study the coordination state of surface-exposed ¹¹B nuclei in MXenes.

Future research in this field could focus on developing new methods for enhancing the sensitivity and resolution of solid-state NMR spectra, as well as combinations of solid-state NMR spectroscopy with other analytical techniques to provide a more comprehensive understanding of 2D materials.

References

[1] Er D., Ghatak K., in *Synthesis, Modeling, and Characterization of 2D Materials and Their Heterostructures,* 2020. P. 243-255.

[2] Reif B., Ashbrook S. E., Emsley L., Hong M., *Nature Reviews Methods Primers*, 2021, 2.

[3] Sun B., Lu Q., Chen K., Zheng W., Liao Z., Lopatik N., Li D., Hantusch M., Zhou S., Wang H. I., Sofer Z., Brunner E., Zschech E., Bon M., Dronskowski R., Mikhailova D., Liu Q., Zhang D., Yu M., Feng X., Redox-Active Metaphosphate-Like Terminals Enable High-Capacity MXene Anodes for Ultrafast Na-Ion Storage. *Adv. Mater.* 2022, 34, 2108682.

[4] Paper submitted: De A., Haldar S., Michel S., Shupletsov L., Bon V., Lopatik N., Ding L., Eng L., Auernhammer G., Brunner E., Schneemann A., Manipulation of Covalent Organic Framework by Side Chain Functionalization - Towards Few Layer Nanosheets. *Chemistry of Materials*.