

Solid-state investigations of 2D Materials

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More than 10 years have passed since the first successful synthesis of graphene. Since then, related two-dimensional materials (2DMs) have attracted increasing interest due to their promising physical, electrical, chemical, and optical properties. 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] The chemical structure and dynamics of solids and semi-solids can be determined with an atomic-level method - solid-state nuclear magnetic resonance (NMR). It has proven to be a versatile technique for studying various materials. ^[2] In this contribution, we investigated two types of 2DMs: transition metal carbides/nitrides (MXenes) and covalent organic frameworks (COFs), using different solid-state NMR experiments.

MXenes is a class of 2DMs with emerging applications in energy storage, electronics, catalysis, and other fields due to their high surface areas, metallic conductivity, biocompatibility, and attractive optoelectronic properties. ^[3] Although MXenes have been noted as attractive fast-charging cation-intercalation electrode materials, they unfortunately suffer from limited specific capacities. The properties of substances are very strongly influenced by their surface chemistry, but understanding the functionalization of the surface remains to be developed. Solid-state NMR spectroscopy is sensitive to the interfacial chemistry and the electronic properties of the MXenes. Herein, we have systematically studied the chemistry of Nb₄C₃T_x/BP and PO_x-Nb₄C₃, using solid-state NMR MAS (magic-angle-spinning) spectroscopy and examined a various of nuclei (¹H, ¹¹B, ¹³C, ³¹P).

COFs are a well-established class of porous and crystalline materials in which organic building blocks are held tightly together by covalent bonds. These porous materials can be used in gas separation, storage (H₂, CH₄) and heterogeneous catalysis. The chemistry of 2D COFs was investigated with solid-state MAS NMR spectroscopy detecting ¹H and ¹³C nuclei by employing techniques, such as CP (cross polarization) and HETCOR (heteronuclear correlation spectroscopy).

References

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