Local Structure in (2D) Energy Materials from Solid State NMR

I will present three examples of how solid-state NMR can selectively determine the atomic-scale structure of emerging functional materials to guide the development of next-generation devices:

- Harnessing the greater polarisation of unpaired electrons in lithium metal using dynamic nuclear polarisation allows selective observation of the metal–SEI interface in lithium metal batteries. This critically determines the nucleation of dendrites, which can short circuit the battery and cause fires. [10.1038/s41467-020-16114-x]

- Layered hybrid perovskites are important surface coatings to extend the lifetime of perovskite solar cells. Isotropic–anisotropic ^{207}Pb NMR demonstrates partial halide ordering in mixed-halide 2D perovskites, which may explain the suppressed halide mobility. [10.1002/anie.202314856]

- MXenes are a class of layered two-dimensional transition metal carbides with promising applications including energy storage and gas separation. NMR reveals the surface functionalisation of these materials, which control the device performance. [10.1039/C6CP00330C, 10.1021/jacs.0c09044]

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Michael is an assistant professor in the Department of Chemistry at the University of Warwick, UK. His research focuses on the use of solid-state NMR and complementary techniques to characterise functional materials at the atomic scale. Michael is particularly interested in materials for energy storage and generation, such as materials for batteries and solar cells, to help combat the growing climate crisis.

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