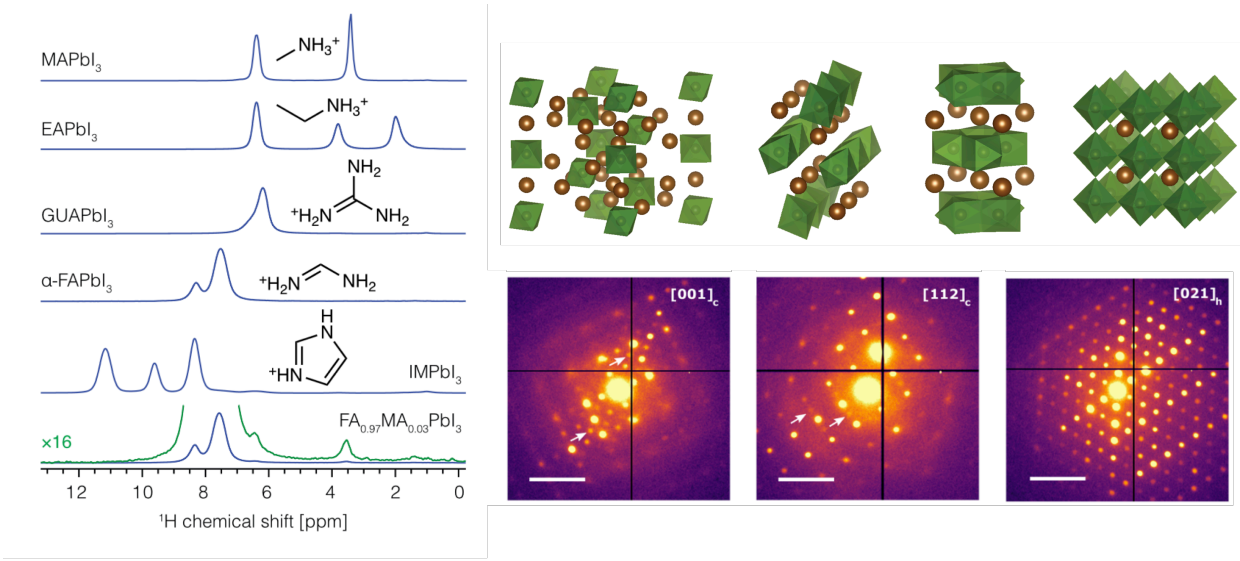
New approaches to determining the atomic-level structure of advanced materials

Determining the structure-property relationships at multiple length scales is one of the key tenets of rational design of new materials. While diffraction techniques offer insight into the long-range structure of solids, many properties are determined by local structure, which can be accessed using approaches based on, e.g., total scattering (PDF), XAFS, and magnetic resonance (NMR and ESR).

I will use the example of metal halide perovskites to discuss how we can determine the atomic-level structure of solids in an element-specific manner using solid-state NMR spectroscopy. The range of research problems includes quantifying dopant incorporation, phase segregation, decomposition pathways, passivation mechanisms, and structural dynamics.[1] I will also show how electron diffraction allows us to study structural phenomena inaccessible with X-rays.[2]

I will then discuss my take on studying these multifaceted materials *in situ* and *operando* to elucidate the mechanism of structural transformations in fully assembled optoelectronic devices, especially under illumination. These strategies will be key to elucidating the performance-limiting factors in devices such as solar cells, light emitting diodes, and X-ray detectors.



References

(1) Kubicki, D. J.; Stranks, S. D.; Grey, C. P.; Emsley, L. NMR Spectroscopy Probes Microstructure, Dynamics and Doping of Metal Halide Perovskites. *Nat. Rev. Chem.* **2021**, *5*, 624–645.

(2) Doherty, T.; Nagane, S.; Kubicki, D. J.; Jung, Y. K.; Johnstone, D. N.; Iqbal, A.; Guo, D.; Frohna, K.; Danaie, M.; Tennyson, E. M.; MacPherson, S.; Abfalterer, A.; Anaya, M.; Chiang, Y.-H.; Crout, P.; Ruggeri, F. S.; Collins, S.; Grey, C. P.; Walsh, A.; Midgley, P.; Stranks, S. D. Stabilized Tilted-Octahedra Halide Perovskites Inhibit Local Formation of Performance-Limiting Phases. *Science* **2021**, *374*, 1598–1605.

Speaker: Dominik J. Kubicki (Department of Physics, University of Warwick)

@DominikJKubicki http://kubickilab.wordpress.com/