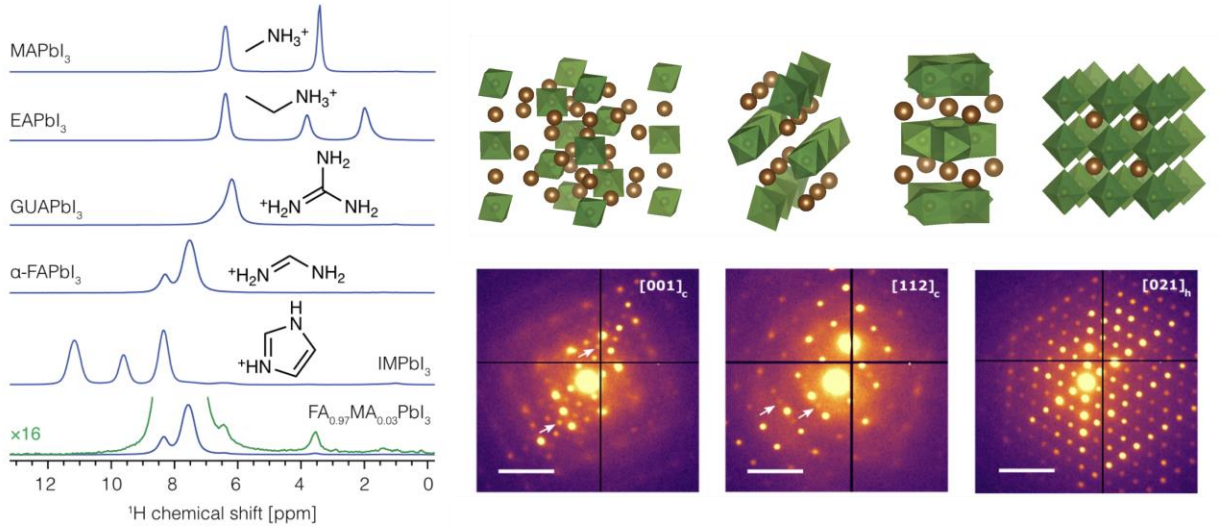
New approaches to determining the atomic-level structure of advanced materials

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.

I hope that sharing these ideas will stimulate a productive and inspiring discussion.



References

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Dominik J. Kubicki is an assistant professor in the Department of Physics at the University of Warwick. He graduated from the Warsaw University of Technology and completed his PhD in solid-state NMR with Lyndon Emsley at EPFL (Switzerland) in 2018. He then worked in the group of Michael Grätzel and subsequently held a Marie Curie-Skłodowska Fellowship at the University of Cambridge working with Sam Stranks and Clare Grey. His research focuses on new materials for sustainable optoelectronic technologies.