

Disorder, Defects and Dynamics in Functional Materials by NMR

Jörn Schmedt auf der Günne, Siegen University, Siegen/Germany

Solid-state nuclear magnetic resonance is an efficient tool to elucidate structure and dynamics of disordered compounds. A simple powerful approach for structural characterization is to study samples synthesized under various conditions by quantitative NMR experiments. In combination with quantum chemical calculations it is possible to identify substitutional defects from their NMR fingerprint [5,6]. Their distribution throughout a host can be studied with multipulse NMR [6] or in case of light-converting phosphors through the *NMR visibility* of the nuclei of the host [1-3]. On the example of inorganic phosphors [1-3], transparent conductive oxides [5,6], anodic aluminium oxide [4] and ionic conductors it is shown, how the NMR toolbox can help to understand the short range order in functional materials.

- [1] W. Li, M. Adlung, Q. Zhang, C. Wickleder, J. Schmedt auf der Günne, A Guide to Brighter Phosphors - Linking Luminescence Properties to Doping Homogeneity Probed by NMR, *ChemPhysChem*. **2019**, *20*, 1–7.
- [2] W. Li, Q. Zhang, J.J. Joos, P.F. Smet, J. Schmedt auf der Günne, Blind spheres of paramagnetic dopants in solid state NMR, *Phys. Chem. Chem. Phys.* **2019**, *21*, 10185–10194.
- [3] W. Li, V.R. Celinski, J. Weber, N. Kunkel, H. Kohlmann, J. Schmedt auf der Günne, Homogeneity of doping with paramagnetic ions by NMR, *Phys. Chem. Chem. Phys.* **2016**, *18*, 9752–9757.
- [4] J.N.M. Aman, J.K. Wied, Q. Alhusaini, S. Müller, K. Diehl, T. Staedler, H. Schönherr, X. Jiang, J. Schmedt auf der Günne, Thermal Hardening and Defects in Anodic Aluminum Oxide Obtained in Oxalic Acid: Implications for the Template Synthesis of Low-Dimensional Nanostructures, *ACS Applied Nano Materials*. **2019**, *2*, 1986–1994.
- [5] Y.S. Avadhut, J. Weber, E. Hammarberg, C. Feldmann, J. Schmedt auf der Günne, Structural investigation of aluminium doped ZnO nanoparticles by solid-state NMR spectroscopy, *Phys. Chem. Chem. Phys.* **2012**, *14*, 11610–11625.
- [6] Y.S. Avadhut, J. Weber, E. Hammarberg, C. Feldmann, I. Schellenberg, R. Pöttgen, J. Schmedt auf der Günne, Study on the Defect Structure of SnO₂:F Nanoparticles by High-Resolution Solid State NMR, *Chemistry of Materials*. **2011**, *23*, 1526–1538.