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In situ neutron diffraction as a guide for chemical synthesis

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Time-resolved *in situ* investigations are very useful for unveiling basic steps of chemical reactions. They are of fundamental importance for many technologically relevant processes, *e. g.* hydrogen storage, electrochemical energy storage or ore smelting, and allow for elucidation of reaction pathways and the identification of intermediates thus enabling better reaction control [1-4]. Neutron diffraction is particularly useful when it comes to light elements such as hydrogen or lithium and has advantages for bulky sample environment due to low absorption cross sections for most elements. Considerations for the design of sample environment allowing for *in situ* neutron diffraction on chemical reactions in the solid as a function of time, gas pressure and flow, temperature, and other external parameters will be discussed [5]. Examples will be given from the areas of research of intermetallic hydrides as hydrogen storage materials [1-3], heteroanionic hydrides as functional materials [6] and ore smelting [7]. A detailed knowledge of the formation conditions has oftentimes proven to be the key to a rational synthesis planning. The chemical synthesis of solids can thus be considerably improved by *in situ* neutron diffraction investigations. Further, it strengthens our fundamental understanding of chemical reactions in the solid state.

- [1] T. C. Hansen, H. Kohlmann, Chemical Reactions followed by *in situ* Neutron Powder Diffraction, *Z. Anorg. Allg. Chem.* 2014, 640, 3044–3063.
- [2] V. K. Peterson, J. E. Auckett, W.-K. Pang, Real-time powder diffraction studies of energy materials under non-equilibrium conditions, *IUCrJ* 2017, 4, 540–554.
- [3] H. Kohlmann, Looking into the Black Box of Solid-State Synthesis, *Eur. J. Inorg. Chem.* 2019, 4174–4180; doi: doi.org/10.1002/ejic.201900733.
- [4] R. Finger, N. Kurtzemann, T. C. Hansen, H. Kohlmann, Design and use of a sapphire single-crystal gas-pressure cell for *in situ* neutron powder diffraction, *J. Appl. Crystallogr.* 2021, 54, 839–846; doi: doi.org/10.1107/S1600576721002685.
- [5] N. Zapp, F. Oehler, M. Bertmer, H. Auer, D. Sheptyakov, C. Ritter, H. Kohlmann, Aliovalent anion substitution as a design concept for heteroanionic Ruddlesden–Popper hydrides, *Chem. Commun.* 2022, 58, 12971–12974; doi: doi.org/10.1039/D2CC04356D.
- [6] M. Häger, S. Keilholz, H. Kohlmann, The reduction of group 6–8 transition metal oxides with hydrogen — from ore smelting to reaction pathways, *Eur. J. Inorg. Chem.* 2025, accepted.

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