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In-situ PDF to reveal molecular complexes and track particle formation

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The pair distribution function (PDF) technique experienced a large revival in recent years in the field of nano-materials as it is able to access the structure of crystallographically challenging materials. [1] By measuring the total, i.e. the Bragg and diffuse, scattering, a variety of materials comprising liquids, glasses and disordered nanoparticles can structurally be analysed. In-situ/-operando PDF experiments can be carried out with a time resolution of seconds to minutes and the high-energy X-rays (50–90 keV) readily penetrate model reactors. This time resolution became possible due to i) the increase in flux at high X-ray energies at synchrotron radiation sources, and ii) novel detector technologies (Pilatus CdTe 1M). Thus recently, not only in-operando insight into batteries under cycling was achieved [2], but we could monitor chemical reactions, bond formation and nucleation processes of nanoparticles. [3] Combined with novel approaches in data processing, we track minute scattering contrasts in-situ to access changes of solvation shells during particle formation.

[1] S. J. L. Billinge, et al., Chem. Commun. 7 (2004) 749

[2] Wiaderek, K. M., et al, J. Am. Chem. Soc. 135 (2013) 4070

[3] M. Zobel, et al., CrystEngComm 18 (2016) 2163

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