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Difference-PDFs of nanostructured interfaces - insight from X-rays and neutrons

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The pair distribution function (PDF) technique has risen to be one of the primary techniques to characterize the atomic structure of nanomaterials, in particular their short-range (dis)order. Nanostructured interfaces in energy materials span, for instance battery materials, nanoparticles in fuel cells and heterogeneous catalysts. In order to access the actual signal of the nanoparticle or interface, the dominating contribution of support materials or adjacent solvents needs to be subtracted. While for ions in solution the neutron PDF technique has paved the ground for interfacial insight quite a while ago, for nanostructured interphases involving typically several phases the situation is more challenging. In this talk, advances in difference-PDF (d-PDF) calculation will be presented which have been established for X-ray PDF on nanoparticle dispersions. The approach of d-PDF calculation is then transferred to neutron PDF touching current limitations and future perspectives.

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