

# **FLAIR** Colloquium

**Institute of Materials Science  
Technische Universität Darmstadt**

**Thursday, 26.10.2023, 16:00**

**Room 2/3, Gebäude L6|01, Otto-Berndt-Str. 3**

**ZOOM Meeting ID: 691 7475 9839**

## ***Atomic Pair Distribution Function (PDF) Analysis***

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Scattering of photons, neutrons, and electrons has long been used to determine crystal structures and how these influence material function. Yet, useful properties in materials often arise as a result of structural disorder, local variations in bonding, composition, microstructure with respect to the periodic crystal structure. Disordered materials produce continuous, diffuse scattering alongside, or even replacing, Bragg peaks. The method of atomic Pair Distribution Function (PDF) analysis, using diffuse scattering as well as Bragg scattering, has emerged as a powerful technique to describe the structure of materials from the local scale to the long-range, irrespective of whether they are amorphous, low-dimensional, nanoparticles, or disordered crystals. This talk will first introduce the PDF function, the real-space function describing the distribution of interatomic distances, and how to obtain it from a “total scattering” experiment. Then, it will give an overview of analytical tools used to interpret the PDF and therefore obtain a structural model of the material investigated. Finally, we will present case studies of PDF analysis being used to determine structural-property relationships in solid state materials, with a particular focus on perovskite titanates and doped cerium oxides.

**Interessierte sind herzlich eingeladen !**

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