Swiss Society for Crystallography

Howard Flack Crystallographic Lecture Series 2023

Local Order and Pair Distribution Function Analysis

Prof. Simon Billinge
Columbia University, New York

Prof. Billinge has more than 25 years of experience developing and applying techniques to study local structure in materials using x-ray, neutron and electron diffraction including the development of novel data analysis methods including graph theoretic, artificial intelligence and machine learning approaches. He earned his Ph.D in Materials Science and Engineering from University of Pennsylvania in 1992. After 13 years as a faculty member at Michigan State University, in 2008 he took up his current position as Professor of Materials Science and Applied Physics and Applied Mathematics at Columbia University and held a joint position of Physicist at Brookhaven National Laboratory between 2008 and 2022.

Prof. Billinge has published more than 350 papers in scholarly journals. He is a fellow of the American Physical Society and the Neutron Scattering Society of America, a former Fulbright and Sloan fellow and has earned a number of awards including the 2022 Distinguished Powder Diffractionist Prize of the European Powder Diffraction Conference, the 2018 Warren Award of the American Crystallographic Association and being honored in 2011 for contributions to the nation as an immigrant by the Carnegie Corporation of New York. He is Section Editor of Acta Crystallographica Section A: Advances and Foundations. He regularly chairs and participates in reviews of major facilities and federally funded programs.

Nanoparticles, nanoporous materials and nanostructured bulk materials are at the heart of next generation technological solutions in sustainable energy, effective new pharmaceuticals, and environmental remediation. Their study involves going beyond traditional crystallography to understand local arrangements of atoms on different length-scales. These lectures will explore this problem, and describe recent developments in solutions based on total scattering methods such as the atomic pair distribution function (PDF) method. They will explore the state of the art in time and spatially resolved studies of heterogeneous samples, *operando* measurements from operating devices, developments in ultra-fast pump-probe PDF measurements using x-ray free electron lasers, and latest approaches in data interpretation using machine learning and artificial intelligence.

The approaches will be illustrated with examples from a wide range of materials science problems from batteries and catalysts, to quantum materials with emergent behaviours, to next generation pharmaceuticals. We will also explore the philosophical question of whether materials have a genome, and if they do, what might we use it for.

Monday 6.11	**EPFL, Sion**
Tuesday 7.11	**University of Bern**
Wednesday 8.11	**University of Basel**
Thursday 9.11	**ETH Zürich**
Friday 10.11	**Dectris AG, Baden** **Paul Scherrer Institute, Villigen**