UNIVERSITÀ DEGLI STUDI DELL'INSUBRIA





Invitation to a Seminar

Prof. Simon J. L. Billinge

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> Wednesday 11.05.2022, at 11:30 Aula Magna @ via Valleggio 11

When hard materials act soft: Local symmetry breaking in bulk materials, how to find it, and why you should care about it.

Modern materials under study for next generation technologies, such as for energy conversion and storage, environmental remediation and health, are highly complex, often heterogeneous and nanostructured. A full understanding of their structure requires us to go beyond crystallography and to study the local structure, which is a major experimental challenge. There are recently emerging powerful experimental developments, for example, using the atomic pair-distribution-function technique (PDF), among others. In this talk, I will focus on bulk materials that have distorted local structures, a potentially large class of materials where, nonetheless, this property has been largely overlooked. In particular, I will focus on materials where atomic or bonding orbitals are electronically active, driving the local atomic distortions. I will describe a new language we are developing for classifying these materials, and new modeling tools that are under development to reveal the local structures. I will also mention areas that need addressing in this endeavor.

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