

# Advanced Simulation Techniques for Total Scattering Data

<http://cnls.lanl.gov/totalscattering>

Total scattering, from neutron and X-ray diffraction, has become a commonly used technique to study the structure of amorphous, disordered and nano-sized materials. This experimental method provides both Bragg and diffuse scattering components, revealing information about the local atomic to long-range structure of materials. In recent years, the use of total energy calculations (such as ab initio and force-field based methods) in conjunction with these experimental tools has emerged as a powerful means to reveal the atomistic nature of increasingly complex materials. These methods are uniquely capable of replicating total scattering data (in reciprocal and real-space) whilst remaining energetically feasible. The Center for Nonlinear Studies at Los Alamos National Laboratory is organizing a workshop exploring the synergy between total scattering and various forms of total energy calculations used to simulate complex materials.

The goal of the workshop will be to provide attendees with an opportunity to discuss current limitations in methods for modeling total scattering data and potential directions forward.

## Session Topics:

- Complex disordered materials and nanoparticles
- Current trends in total scattering modeling and simulation techniques
- Ab initio and force-field based simulations of complex materials
- Examples of combining experiment and theory (including dynamics)
- Software development

## Tour:

On October 16th, there will be a tour of the Lujan Neutron Scattering Center at LANSCE. US and non-US citizens are invited. Register online for more information.

## Important Dates:

Contributed Talk Submissions - August 24th  
Early Registration - September 19th

**October 16-19, 2012**  
Santa Fe, New Mexico, USA

## Confirmed Speakers

Simon Billinge  
Columbia University

Martin Dove  
University of London

Takeshi Egami  
University of Tennessee and ORNL

Mark Johnson  
Institut Laue-Langevin

Alex Navrotsky  
University of California, Davis

Daniel Shoemaker  
Argonne National Laboratory

## Organizers:

Mark Johnson, ILL, France  
Thomas Proffen, ORNL  
Claire White, LANL