Dr. Claire White

Los Alamos National Laboratory

is the recipient of the

2012 Prize for Outstanding Student Research

of the Neutron Scattering Society of America (NSSA) with the citation

"For pioneering a new methodology to elucidate accurate structural representations of complex materials by combining neutron diffraction and computational chemistry"

Dr. Claire White

The Neutron Scattering Society of America (NSSA) established the Prize for Outstanding Student Research to recognize *outstanding accomplishments in the general area of neutron scattering by graduate or undergraduate students who have performed much of their work at North American neutron facilities.* The prize was established in 2011 and will be awarded for the first time.

The nominations were reviewed by a committee of experts in the field of neutron science and the NSSA is pleased to announce that the recipient of the 2012 Prize for Outstanding Student Research is **Dr. Claire White** of the Los Alamos National Laboratory. The prize and $1000 honorarium will be awarded at the 2012 ACNS in Washington, DC, June 24-28, 2012 (http://www.mrs.org/acns-2012/).

Ordinary Portland cement-based (OPC) concrete is the most used building material world-wide and is the 2nd most used resource, after water. However, concrete is the 3rd highest CO_2 emitter, accounting for 5-8% of all man-made emissions, and therefore there is massive scope for technological development of alternative concretes. During her graduate studies Dr. White pioneered a new methodology to elucidate accurate structural representations of complex materials by combining neutron diffraction and computational chemistry. She used the disordered aluminosilicate material, metakaolin, an alternative cement precursor, as the case study, with the methodology revealing the existence of III-coordinated aluminum, which has never before been shown to exist in this material. This research exemplified the power of

combining local structural data (i.e., neutron pair distribution function analysis) with first-principles calculations for amorphous materials, especially when used in an iterative manner to maintain thermodynamic feasibility and agreement with experimental data.

Dr. White has also been heavily involved in technique development with respect to incoherent scattering and neutron pair distribution function analysis. For hydrogen and other incoherent scattering elements, the neutron pair distribution function technique is greatly affected, reducing the ability to obtain high quality PDFs. During her graduate studies, including the 8 months spent at the Lujan Neutron Scattering Center in 2009, Dr White participated extensively in the development of new tools capable of subtracting out the incoherent scattering component of total scattering data.

Dr. White graduated from The University of Melbourne in November 2010, and is currently a Director's Postdoctoral Fellow at Los Alamos National Laboratory with a joint appointment involving the Lujan Neutron Scattering Center and the Theoretical Division. Her research involves combining theoretical and experimental techniques to advance the understanding of low CO_2 cements (geopolymers) and associated materials. Furthermore, she is active in the area of technique development and is constructing novel methodologies combining experimental data and simulations.