COLOQUIO DE FÍSICA

UNIVERSIDAD DEL VALLE
Departamento de Física&
Posgrado en Ciencias-Física

Semestre II de 2013

Celebración 50 años de la Creación del Depto. de Física

Energy Landscape in Frustrated Systems: Cation Hopping and Relaxation in Pyrochlores

Juan Claudio Nino

UFRF Professor, Department of Materials Science and Engineering

University of Florida, Gainesville

USA

We present the dynamics of the local environment and electronic structure in inherently dipolar frustrated pyrochlore compounds to help identify the fundamental nature of dipolar disorder in pyrochlore systems and determine the necessary and sufficient conditions for dielectric relaxation. We map out the energy landscape associated with cation hopping events in three compounds and correlate the hopping pathway with experimental dielectric response. In addition, we present a detailed comparison of the vibrational modes and relaxation behavior in Bi2Ti2O7 (BTO), Ca1.5Ti1.5NbO7 (CTN), and Bi1.5ZnNb1.5O7 (BZN). Through comprehensive analysis of this combined experimental and computational work, rules to predict the occurrence of relaxation and cation hopping pathways will be postulated.

Septiembre 19 de 2013, 11:00 AM, Sala de Conferencias del Departamento de Física
Edificio de Ciencias Naturales y Exactas, Espacio 320-2182