DIRECTION DES SCIENCES DE LA MATIERE,
INSTITUT RAYONNEMENT MATIÈRE DE SACLAY

SERVICE DE PHYSIQUE ET DE CHIMIE DES SURFACES ET DES INTERFACES

SEMINAIRE

Vendredi 5 Juillet 2013 à 11h00

Bâtiment 466, salle 111 - CEA Saclay, 91191, Gif sur Yvette

Finite-temperature properties of Ba(Zr,Ti)O3 relaxors from first principles

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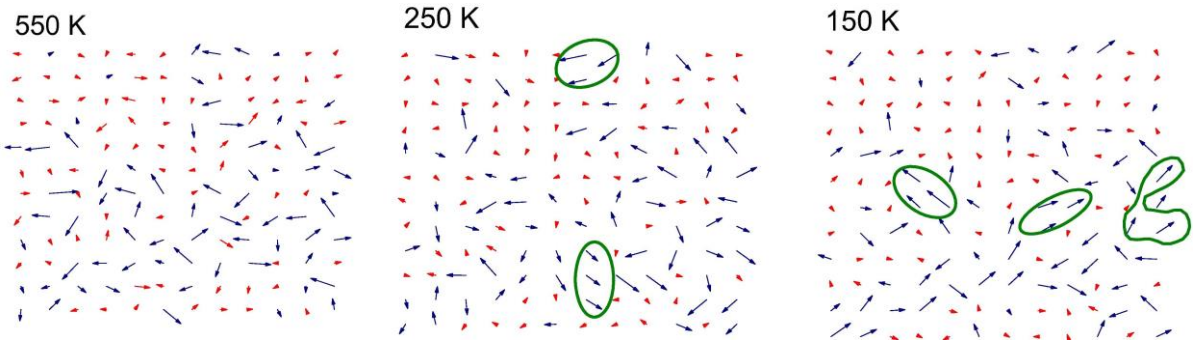
(invité par Nick BARRETT)

Relaxor ferroelectrics are characterized by some striking anomalous properties. For instance, they adopt a peak in their ac dielectric response-versus-temperature function while they remain macroscopically paraelectric and cubic down to the lowest temperatures. Furthermore, this dielectric response deviates from the "traditional" Curie-Weiss law for temperatures lower than the so-called Burns temperature. Other examples of anomalous properties include the plateau observed in their static, dc dielectric response at low temperature, and the unusual temperature behavior of the Edwards-Anderson parameter. Determining the origin of these intriguing effects has been a challenge to scientists for more than half a century. Moreover, many other questions remain opened for discussion. Examples of such questions are: what do the different critical temperatures usually found in relaxors correspond to? Do polar nanoregions really exist in relaxors? If yes, do they only form inside chemically-ordered regions? Is it necessary that antiferroelectricity develops in order for the relaxor behavior to occur? Are random fields and random strains really the mechanisms responsible for relaxor behavior? If not, what are these mechanisms?

Motivated to resolve such questions and to better understand relaxors, we decided to study disordered Ba(Zr0.5Ti0.5)O3 (BZT) solid solutions, via the development and use of a first-principles-based effective Hamiltonian. Interestingly, our ab-initio-based calculations not only reproduce the anomalous features of relaxors but also offer a deep microscopic insight into BZT. Such insight allows to answer the aforementioned questions, and will be discussed in detail during this talk.



Snapshots of dipolar configurations in Ba(Zr,Ti)O3 relaxors for different temperatures

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