Appunti di Fisica '17
&
Dottorato di Ricerca in Fisica

23 maggio ore 15:00
Aula Magna, Incubatore d'Impresa (piano terra)

Modelling Ionic Conductivity in Materials. Glasses, Ionic Liquids and Ionogels

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In this talk, I will present in brief the MIGRATION concept which was developed for modelling conductivity and permittivity spectra of materials with structural disorder. The model formulation generates a time-dependent correlation factor using simple physical picture to describe relaxations following an ionic hop in a dynamically varying potential landscape. Using linear response theory, this function can be Fourier transformed to yield scaled model conductivity and permittivity spectra. The model parameters help us examine features of spectra such as the shape of the spectra, scaling, length scales for localised diffusion, and temperature-dependence of DC conductivity. A few examples where the model has been successfully employed to understand ion transport will be given.

As part of my ongoing NEWFELPRO project, I examine these features in mixed glass former systems where we can correlate local structure obtained from Raman and NMR techniques to the spatial extent of local hops of the ion. In ionic liquids, both neat and contained in supramolecular gelator matrix, the shape of the spectra is first modelled. Using this, one can model the high-frequency conductivity and extract the activation energy of elementary displacements. This helps in modelling DC conductivity, and in constructing model conductivity isotherms. Remarkably, even

in iron phosphate glasses which show polaronic conduction, the MIGRATION concept has been able to provide insights, revealing that the model is applicable whether the hopping species is an ion or an electron, since the hop produces disturbance in the neighbourhood in the form of a polarising field. Insights gleamed from this are discussed.

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