NAPLES, ITALY 23-27 JUNE
DSL2025 NAPLES
21st International Conference on Diffusion in Solids and Liquids

ABSTRACT

Exploring Deep Eutectic Solvents: What Insights Can Inelastic Neutron Scattering Spectroscopy Provide?

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The study of deep eutectic solvents (DES) has become a key area of interest in contemporary chemistry due to their unique properties and potential applications. A "deep eutectic" refers to a mixture with a melting point lower than that of its individual components. This occurs because new intermolecular interactions form between the DES components—typically a hydrogen bond donor (HBD) and a hydrogen bond acceptor (HBA)—resulting in negative deviations from ideal behavior.
Our work relies on the use of vibrational spectroscopy data from Infrared (IR), Raman and Inelastic Neutron Scattering (INS) techniques to assess the systems experimentally. Simulations using both discrete and periodic models are used to describe and assess the experimental systems in an iterative process. This falls under the concept of Computational Spectroscopy (CS) where one can use information from experimental vibrational spectroscopy data to build structural models that are more realistic and can be validated by simulation data than more orthodox approaches. This is particularly relevant in situations where crystallographic structures are unavailabe.

The combination of inelastic neutron scattering (INS) spectroscopy and periodic density functional theory (DFT) calculations provides valuable insights into various aspects of deep eutectic solvents, such as the role of water [1] and the influence of entropic factors on their behavior [2].

[1] M. M. Nolasco, S. N. Pedro, C. Vilela, P. D. Vaz, Paulo Ribeiro-Claro, S. Rudić, S. Parker, C.S.R. Freire, M. G. Freire, A. J. D. Silvestre. Frontiers in Physics 10, 834571 (2022)
[2] C.F. Araujo, P. Ribeiro-Claro, P.D. Vaz, S. Rudić, R. Serrano, L.P. Silva, J.A.P. Coutinho, M.M. Nolasco, Physical Chemistry Chemical Physics, 26, 5969 (2024)