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Vibrational spectroscopies insights on the molecular interactions in Deep Eutectic Solvents: a step forward in the rational design of electrolytes for energy devices

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Since their discovery, Deep Eutectic Solvents (DES) have been gaining growing attention due to their versatility coupled with good sustainability[1]. Indeed, DES are usually formulated starting from inexpensive, abundant and renewable materials. Initially, they were made by the complexation of choline chloride (ChCl, a quaternary ammonium salt) with a Hydrogen Bond Donor (HBD), which usually was urea, a carboxylic acid, a polyalcohol or a metal salt. Even though more than 15 years have passed since their discovery, fundamental research on these mixtures is still in its infancy. As a matter of fact, scientists mainly focused their efforts on the final application of DES.[2] Indeed, they were successfully employed in metal processing and extraction, as green solvents or gas absorbers and in industrial applications. The replacement of ChCl with metallic salts (e.g. NaCl, ZnCl2⋯) will enable their exploitation as electrolytes for electrochemical energy storage systems. Notwithstanding the broad application of DES, a thorough knowledge of the chemical and physical interactions lying behind their formation is necessary, especially when one of the components is liquid at room temperature.[3] In fact, the solubilization of the salt in a liquid HBD could lead to either a DES or a salt-in-solvent system, following on from the intermolecular interactions established.
In this context, a stable hydrogen bond network (HBN) seems to play a pivotal role in the formation of the supramolecular interaction characterizing a DES. Recently, we explored the use of spectroscopy (both IR and Raman) coupled with structural and electrochemical analyses to analyze the HBN of a couple of mixtures of metal salts and glycerol: data analyses, supported by computational calculation, allowed us to determine the eutectic composition unequivocally.[4] However, lab-scale instrumentation usually suffers from low sensibility at lower wavenumber (< 150 cm-1), preventing us from systematically analyzing how the HBD nature influences the energetic contribution of HBN in DES formation. Here, the exploitation of advanced spectroscopic techniques, especially Far-InfraRed, provided at the Elettra synchrotron could allow a dramatic improvement in the fundamental understanding of the HBN in DES. Moreover, the rationalization of the dynamics and the energy of the HBN would be fundamental to designing stable liquid systems as electrolytes in electrochemical storage systems (i.e. batteries and supercapacitors).

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