# Modeling Spectral Signals of Molecular Systems Dissolved in Deep Eutectic Solvents

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Nowadays, every field of chemistry is engaged in the research of more sustainable and greener processes to reduce the environmental impact of chemical industry activities. In this context, Deep Eutectic Solvents (DESs)[1] have gained in the past few years enormous consideration as an environmental-friendly alternative to ionic liquids (ILs) and their applications have been extended to many areas of chemistry from pharmaceutical studies to industrial processes[2]. Since DESs are primarily used as solvents, understanding how molecular systems behave in such media is therefore a fundamental step in the comprehension of these environments.

Here, we adapted a computational protocol[3] widely used to investigate spectroscopic properties in aqueous environments to calculate the absorption spectrum of hydroxymethylfurfural (HMF) in choline chloride/ethylene glycol (ChCl/G). Solvation effects acting on the solute molecule are taken into account via multiscale/focused models[4]. In particular we exploit Quantum Mechanical (QM)/Molecular Mechanics (MM) models[5], in which the solute responsible for the spectroscopic signal is treated at the QM level whereas the solvent is described by classical force fields. These models explicitly consider the solvent molecules and are able to capture the solute-solvent electrostatic interactions and hydrogen bonding[3]. These models, coupled with a phase-space sampling method as classical molecular dynamics (MD), are able to take into account also the dynamic aspect of the solvation phenomenon. It will be shown the whole procedure with particular attention to solute-solvent coupling and finally a comparison with preliminary experimental data is discussed.

References:

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