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Nerea Rodriguez Rodriguez [C, S], Marisa A. A. Rocha and Maaike C. Kroon
Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, Eindhoven, Netherlands
n.rodriguez@tue.nl

Ionic liquids (ILs) have been successfully tested in a wide range of applications; however, their high price and complicated synthesis make them infeasible for large scale implementation. A decade ago, a new generation of solvents so called deep eutectic solvents (DESs) was reported for the first time. DESs show similar properties to ILs and they have proven to be an excellent alternative to ILs in many applications where ILs succeeded first. Besides, DESs can be prepared easily and cheaply, with low-cost starting materials, no need of solvents, no atom loss during the formation and no additional purification requirements. The main problem that scientist are facing when they want to use DESs in different applications is the lack of information on the fundamentals of these solvents. Why do they form? How do they form? How do the hydrogen bond donor (HBD) and the hydrogen bond acceptor (HBA) interact? How do DESs interact with other compounds? Can we predict their thermophysical properties? The answer to these questions will provide to researches new insights on the application of these solvents, solving the problem of trial-and-error experimentation. In this work, we present a detailed analysis of molecular interactions and conformational states of two selected DESs: lactic acid – choline chloride (2:1) and glycolic acid – choline chloride (1:1), using density functional theory (DFT) and second-order Møller–Plesset perturbation theory (MP2) with various basis sets. Theoretical calculations were performed using the GAUSSIAN 03 software package. The obtained results are used to evaluate the nature of interactions between the HBD and HBA and their structural features. Additionally, it will contribute to the better understanding of how DESs are formed.