Structural solvation features in novel solvent media.

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Solvation is a fundamental process characterizing a variety of technologically relevant processes. It represents an essential bridge between microscopic features of solvents and the overall thermodynamic, structural and dynamic macroscopic properties of solutions. Its exploration is of paramount importance, especially when considering the new generations of solvent media that have been proposed over the last couple of decades, including ionic liquids, (deep) eutectic solvents (DES) and low transition temperature mixtures (LLTM).

These novel media often represent breakthrough in terms of macroscopic performances, due to their specific and targeted solvation capabilities towards a variety of substances, including biomass, (bio) macromolecules, organic compounds and drugs.

In this contribution, I will report on our recent studies on a variety of solvents and on the detailed nature of their solvation capabilities, exploiting the synergy between experimental (X-ray or neutron scattering) and Molecular Dynamics simulations. This research approach looks quite relevant to explore solvation features, as both tools provide direct access to microscopic structural and dynamic scales (nm / nsec), thus accessing the very details of microscopic interactions that lead to efficient solvation.

I will cite recent results on the development of new, water based DES[1,2] and on their capability, similarly to reline, the prototype DES, to solvate complex carbohydrates, such as cyclodextrins (CD). Therein, the balance between hydrogen bonding and dispersive interactions turns out to be fundamental to stabilize CDs against flocculation. [3–5]

I will also report on recent results on newly developed, eco-sustainable LLTMs, which can efficiently dissolve polyethylene-terephthalate (PET) and illustrate the microscopic mechanism of solvation.

References

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