Computer simulation of solvent properties

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The properties of various liquids, ranging from water, alcohols and organic solvents to ionic liquids, have been a research topic of long standing interest. Determining observables such as diffusion constants, densities, conductivities, dielectric spectra or solvation dynamics can nowadays easily be done on the computer. The role and application of molecular dynamics simulations employing classical or polarizable force fields, as well as quantum-mechanical calculations are comprehensively discussed in this talk. To this aim, recent developments within computational solvation dynamics in bulk solvents [1,2] and close to biomolecules [3,4], as well as dielectric spectroscopy [5] and the design of polarizable force fields [6] are highlighted.

References:

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[5] E. Heid, B. Docampo-Alvarez, L. M. Varela, K. Prosenz, O. Steinhauser and C. Schröder, *Phys. Chem. Chem. Phys.* **20** (2018), 15106.

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