The true nature of the solution phase: hybrid approaches of quantum chemistry, statistical mechanics and kinetics for chemical condensed phase

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As the number of molecules increases and the size of the molecules increases, the number of degrees of freedom composing the system increases. A well-known “more is different” is a key to understanding the diversity of materials, often manifested through the cooperativity inherent in the ensemble of molecules. We are devoted to studying mainly condensed chemical systems composed of polyatomic molecules. In particular, the research focuses on chemical processes in solution by developing several new hybrid approaches of quantum chemistry and statistical mechanics for molecular liquids. The RISM-SCF-SEDD is a representative, combining integral equation theory for molecular liquids (RISM) and quantum chemical calculations. This method is slightly computationally demanding to PCM. Still, it can provide solvation information at the molecular level, like the QM/MM method, applied to various chemical phenomena. In this talk, we will report one of the recent progress, including NMR theory based on RISM-SCF-SEDD/RISM-SCF-cSED to calculate the chemical shifts of molecules in solution.

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