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Insight from first principles: Embedding Techniques, Rate and Thermodynamic Changes, Solvation Effects, and Chiral Polaritonics

Tuesday 3 October 2023 09:00 (40 minutes)

Various experiments have demonstrated that strong collective interaction influences chemical reactivity – it remains to build a conclusive understanding.
Certain aspects such as a resonant behaviour, specific trends in the thermodynamic observables, and a strong sensitivity to the solvent have been identified as critical.
Capturing those effects in a consistent theoretical model is challenging. Here, we will discuss the beneficial use of ab initio quantum electrodynamics, embedding techniques [3,4], and machine learning [2]. Specific observations include cavity induced resonant changes in rate, enthalpy, and entropy that are qualitatively consistent with experiment [1,2] and changes in the local solute-solvent behaviour induced by collective strong coupling [5]. Lastly, we discuss the consequences of breaking chiral symmetry with specifically designed electromagnetic environments, thus suggesting a new direction for polaritonics and chiral recognition [6,7].

References:

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[6] C. Schäfer, D. Baranov, J. Phys. Chem. Lett. 2023, 14, 15, 3777-3784.
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