Quantum Solvation: Hydrogen-Bonding and Chemical Reactions in Superfluids

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Ab initio path integral simulations provide a perfect numerical framework to study nuclear quantum effects in chemically complex systems including chemical reactions thus making and breaking covalent bonds. We recently extended our method such that reactive molecules and microsolvated clusters can be embedded in superfluid environments. I will sketch our ab initio/bosonic PIMD/PIMC hybrid method as implemented in the `CP2k` program package and discuss some showcase applications.