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# Observing solvation free energy changes during biological processes with THz spectroscopy

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Water is much more than a passive spectator during biological processes, such as enzyme-substrate binding, proteins folding and liquid-liquid phase separation. Solvation entropy and enthalpy changes actively contribute to shape the free energy landscape, together with the contributions from biomolecules interactions and entropy. Usually, the partial entropic and enthalpic solvation terms are large, but compensate each other with a subtle entropy/enthalpy balance, resulting in small free energy differences that can be tuned with small adjustment of the environment (e.g. temperature, concentration, co-solutes). However, a rational tuning requires mapping the complex interplay of local hydrophobic and hydrophilic solvation contributions. This remains a challenge for both theory and experiments, and cannot be achieved by standard calorimetry.

In this talk, I will present a novel approach, called THz-calorimetry, to quantify the solvation entropy and enthalpy changes during biological processes directly from experimentally measured THz spectra.1 The main advantages are two: (i) the THz spectra can be recorded as a function of time, with time resolutions down to ps, allowing to follow the free energy changes during chemical processes in real-time; (ii) we can dissect and interpret the thermodynamic quantities by deconvolving the THz spectra into local solvation contributions. In particular, the low frequency THz range is ideal to probe solvation, and I will show that the THz spectra systematically contain two well-separated signatures from water hydrating hydrophilic and hydrophobic groups. THz-calorimetry allows a quantitative correlation of the partial amplitude of these two spectroscopic contributions with partial ΔH and ΔS contributions from hydrophobic and hydrophilic hydration. I will illustrate the relevance of this approach to quantify and interpret solvation effects in biological processes with two applications: liquid-liquid phase separation of alpha-elastin2 and host-guest interactions between a biologically-inspired supramolecular catalyst and its substrate.3

References

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