

Ultrafast exchange dynamics of electrolyte in Lithium ion battery

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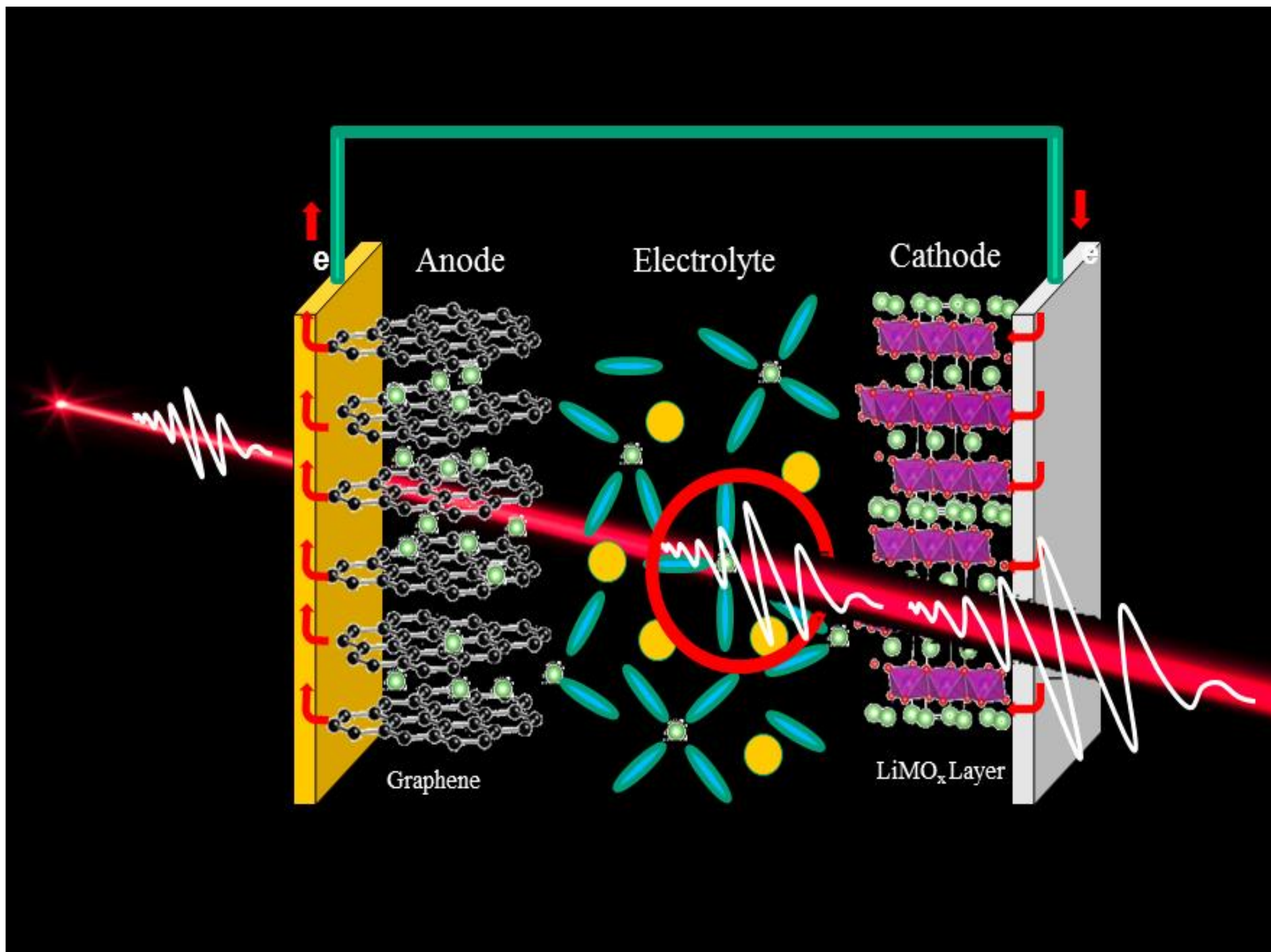


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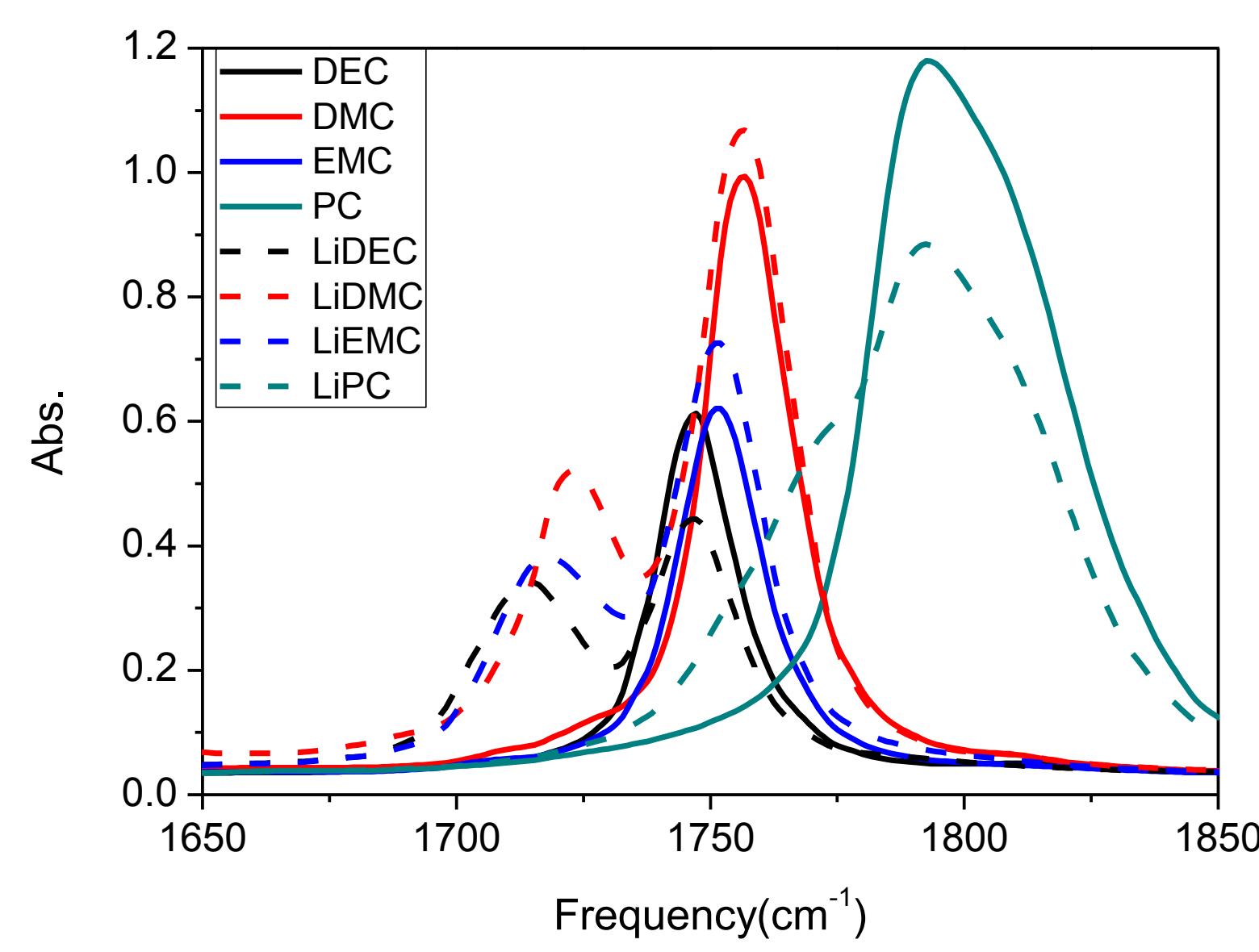
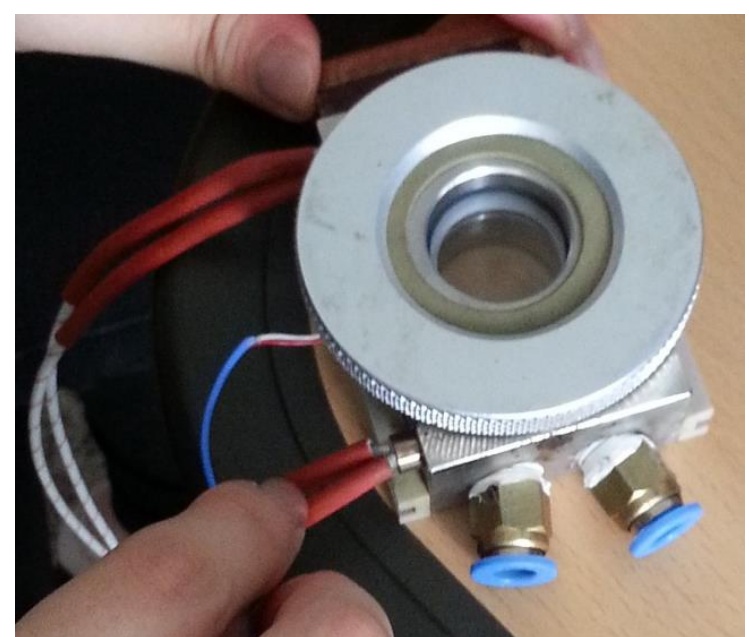
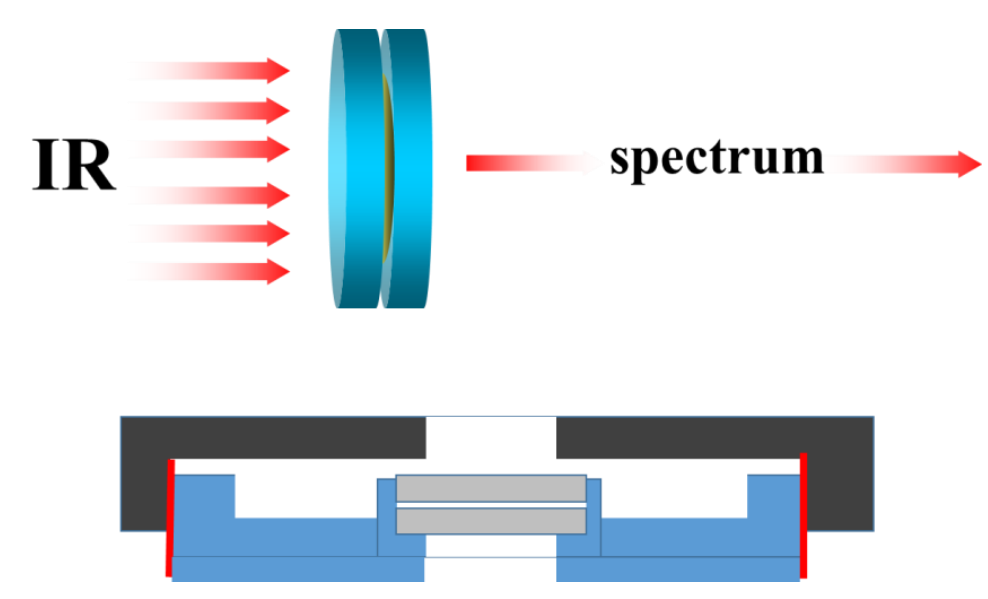
Concept



- Target : electrolyte system in lithium ion battery
- Experimental technique: Ultrafast 2DIR spectroscopy, IR Pump-Probe spectroscopy
- A study ultrafast dynamics of around lithium ion in electrolyte solution with 2DIR & IR PP technique

Electrolyte in lithium ion battery

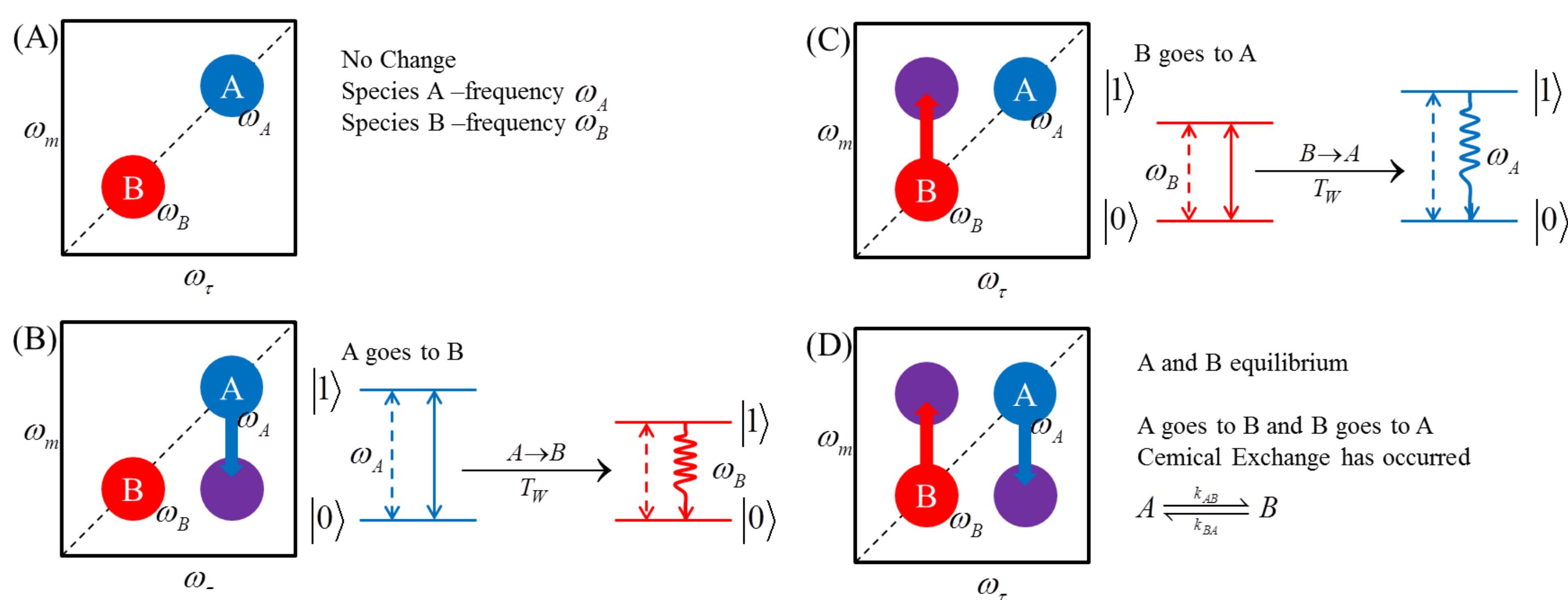
© Home-made cell to overcome saturation



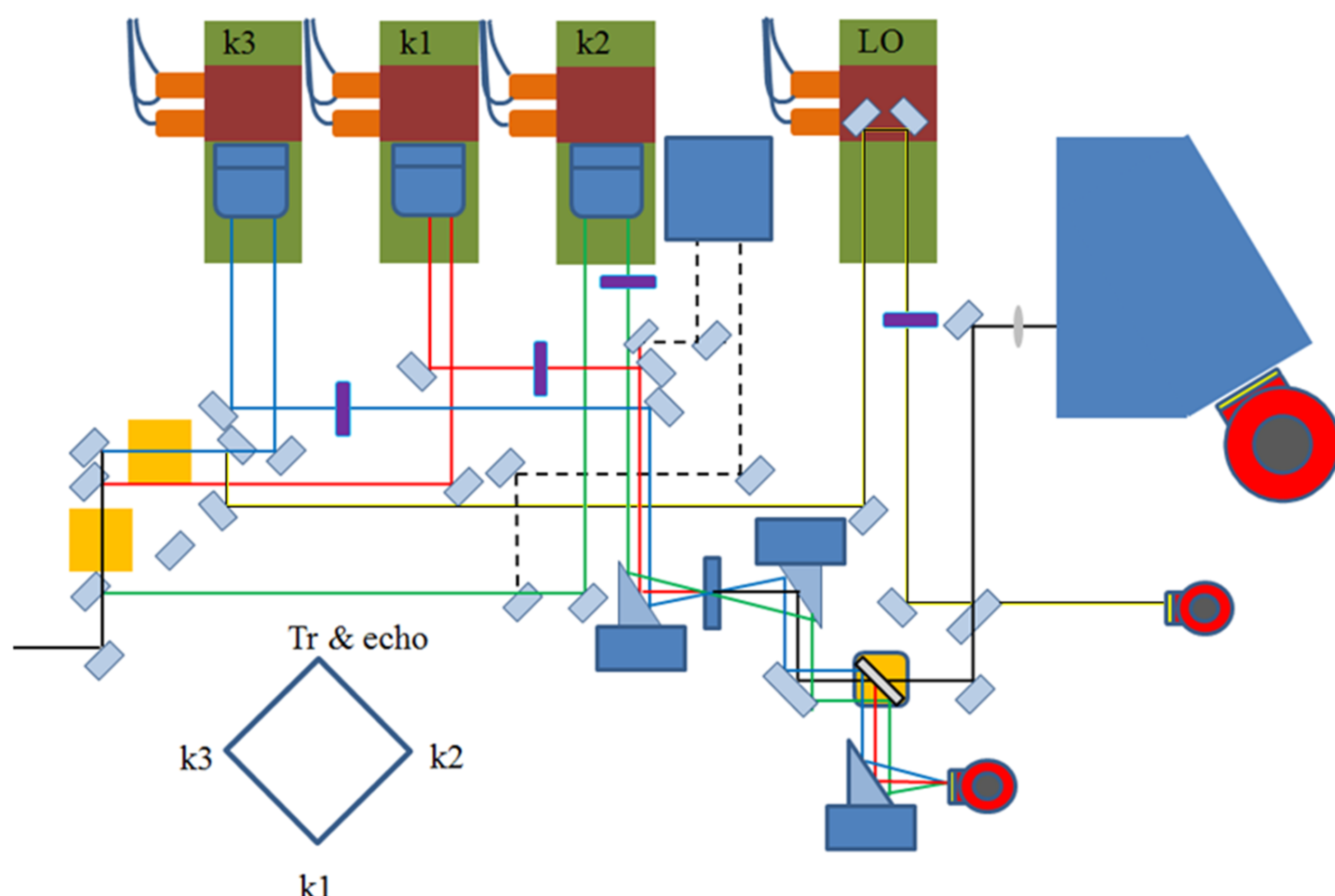
- Electrolyte solutions used in LIB are composed of non-aqueous carbonate solvents and lithium salt.
- Low frequency peaks can be assigned to the C=O stretch modes of carbonate molecules directly interacting with Li⁺.
- Infrared probe is also the solvent, its linear absorption is saturated with normal cell.

Experimental Method

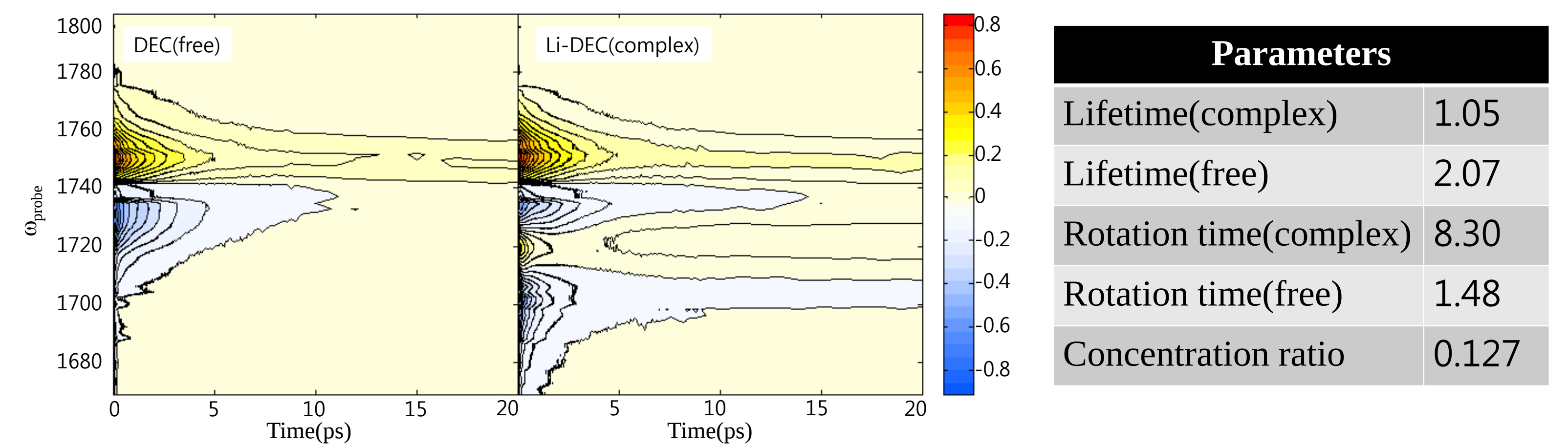
© Chemical Exchange dynamics with 2DIR spectroscopy



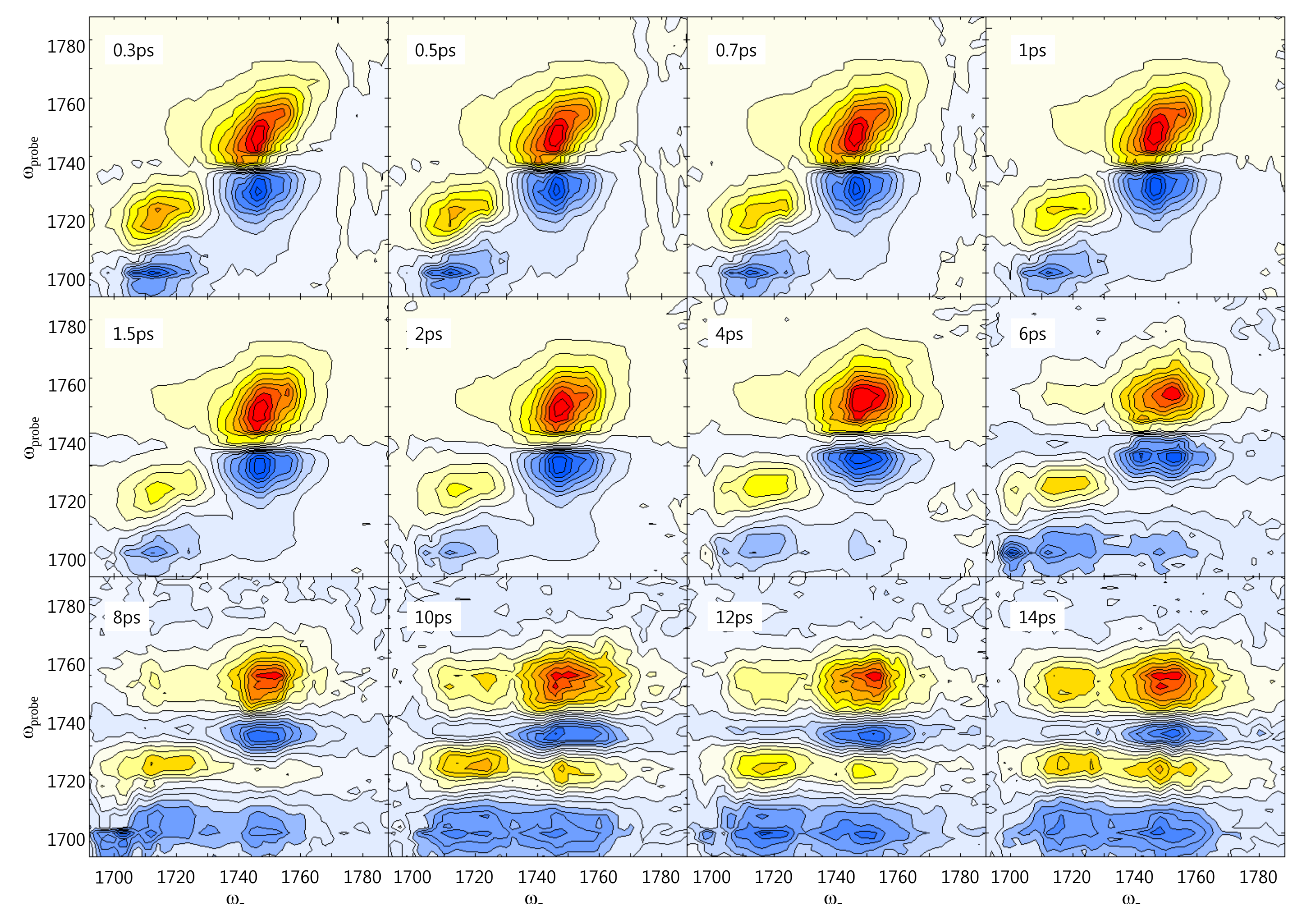
© Experimental scheme of 2DIR spectroscopy



Result

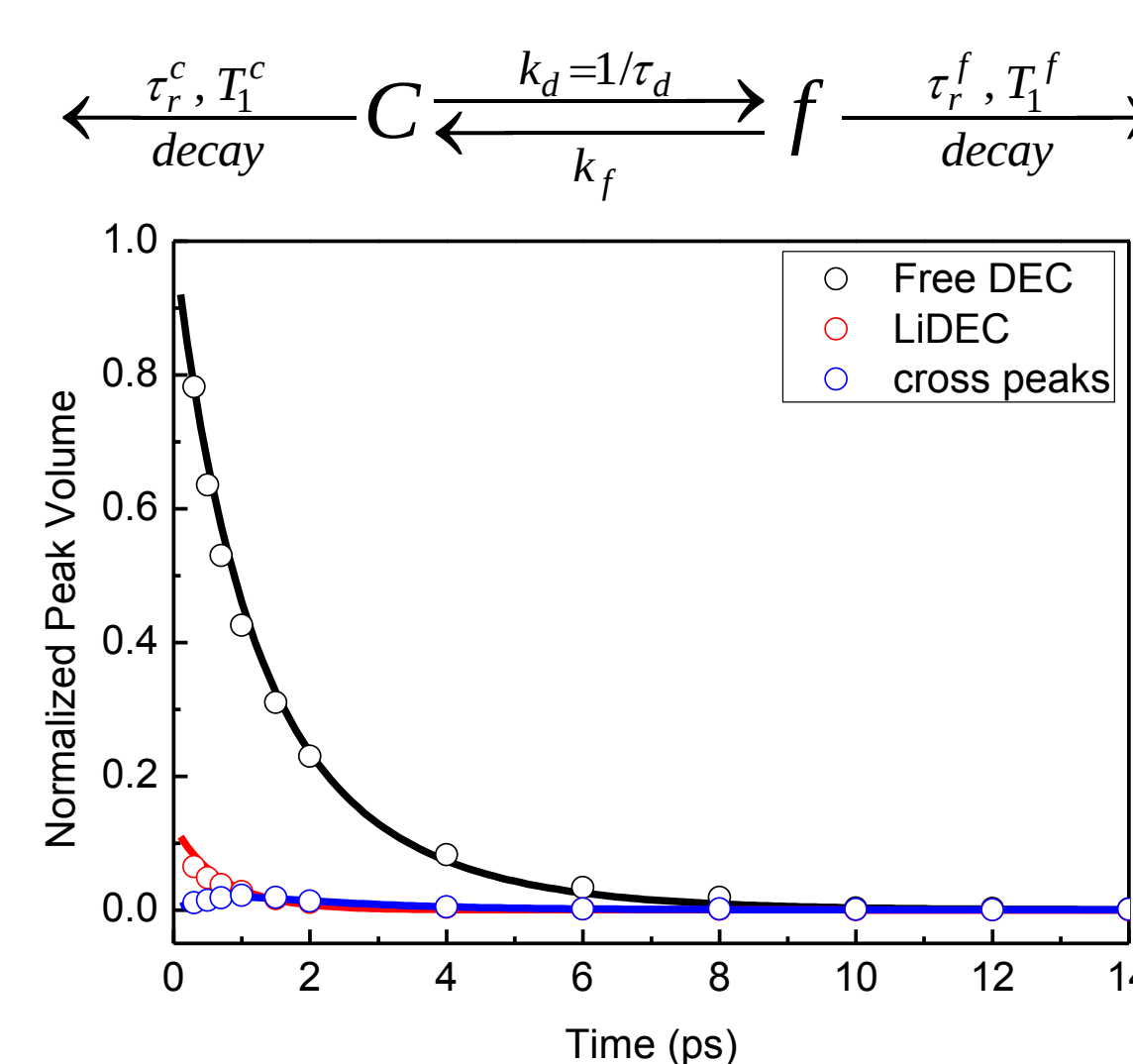


- The vibrational lifetime could be extracted from the fitting analysis of the 1–2 transition PP data that are relatively immune to local heating effect.
- The corresponding time constants of free DEC were obtained from the excited state absorption signal in the infrared PP data of pure DEC solvent.



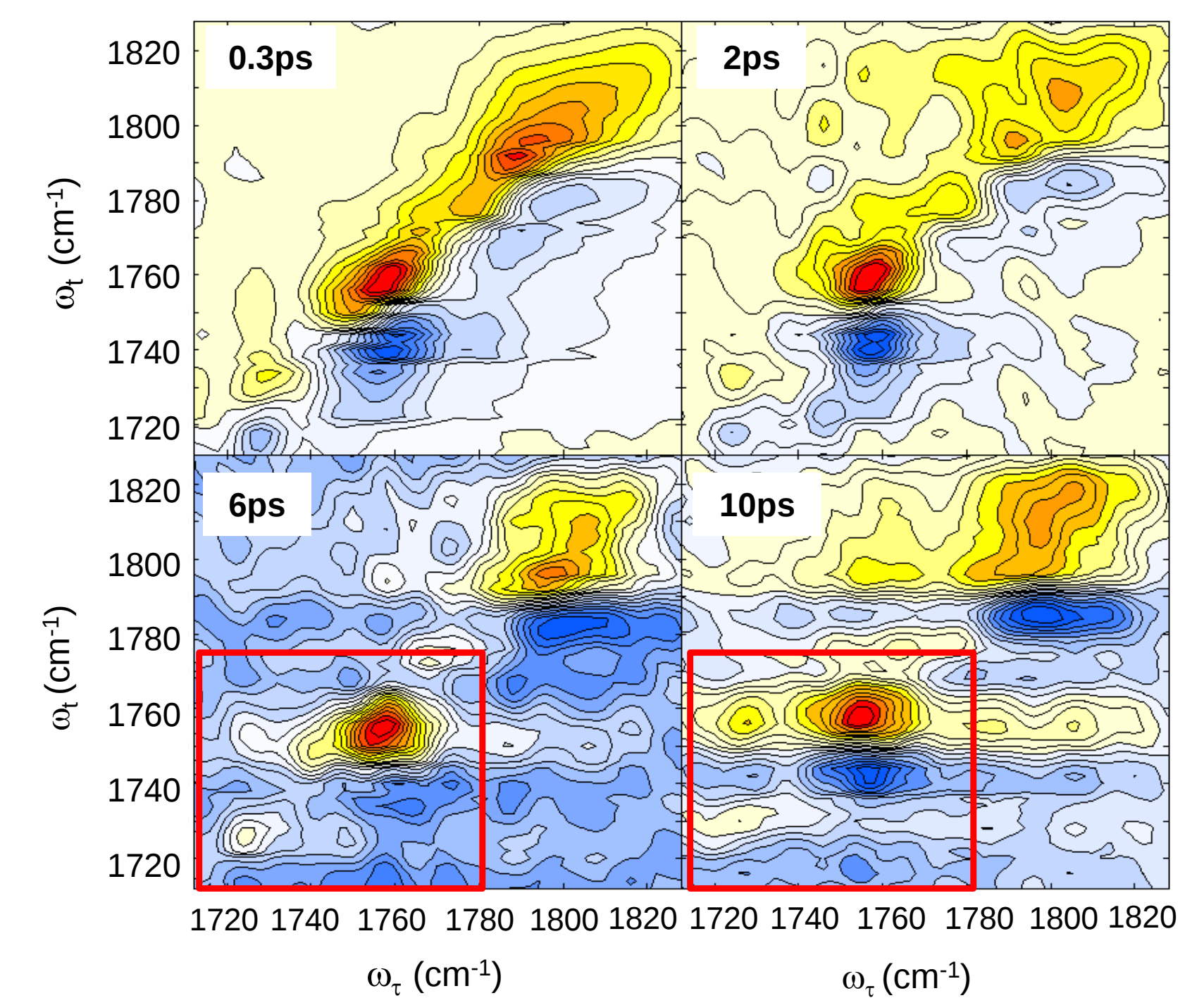
- At a very short waiting time, there are only two peaks on the diagonal line which correspond to the two absorption peaks in the FTIR spectrum.
- At longer waiting time, one can clearly observe cross peaks, that is breaking and forming dynamics between lithium ion and carbonate solvent.

© Chemical exchange



Dissociation time $\tau_d = 2.2$ ps

© 2DIR of electrolyte in mixed solvent



Conclusion

- We could control the thickness of coated SiO₂ layer on CaF₂ window for linear and nonlinear infrared spectroscopic studies.
- Lifetime of free DEC is almost independent of LiPF₆ concentration
- 2DIR spectroscopy clearly shows ultrafast fluxional changes of Li⁺ solvation in LIB electrolyte solutions.
- We could observe measurable diagonal and cross peaks in our 2DIR spectra in mixed solvent system.

Acknowledgment

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