

The study of salt effect on water network in THz region: KSCN vs NaCl

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The THz spectroscopy is sensitive technique that can investigate their collective motions. THz spectroscopy is corresponding to intermolecular interaction while general Mid-IR is related with intramolecular vibration. So this technique can provide different aspects to us. And classical MD simulation revealed separated contribution for total absorption what is dominated contribution. Using two systems, KSCN and NaCl solution within solubility limit, we investigated relative intensities of each species, they showed not only clear concentration dependence but also the effect of cross correlation term which occupies significant amount between ions at high concentration.

References

- [1] Kim, S. H.; Kim, H. J.; Choi, J. H.; Cho, M. H. Ion aggregation in high salt solutions: Ion network versus ion cluster. *J. Chem. Phys.* **2014**, *141*, 124510.
- [2] Schmidt, D. A.; Birrer, O.; Funkner, S.; Born, B. P.; Gnanasekaran, R.; Schwaab, G. W.; Leitner, D. M.; Havenith, M. Rattling in the cage: Ion as probes of sub-picosecond water network dynamics. *J. Am. Chem. Soc.* **2009**, *131*, 18512-18517.
- [3] Funkner, S.; Niehues, G.; Schmidt, D. A.; Heyden, M.; Schwaab, G.; Callahan, K. M.; Tobias, D. J.; Havenith, M. Watching the low-frequency motions in aqueous salt solutions: The terahertz vibrational signatures of hydrated ions. *J. Am. Chem. Soc.* **2012**, *134*, 1030-1035.