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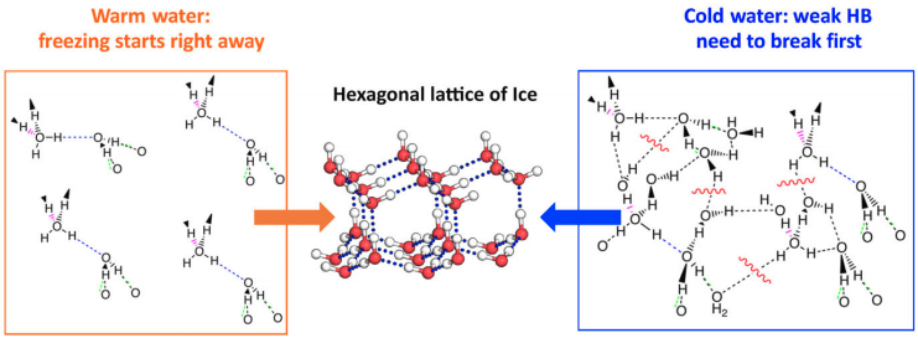
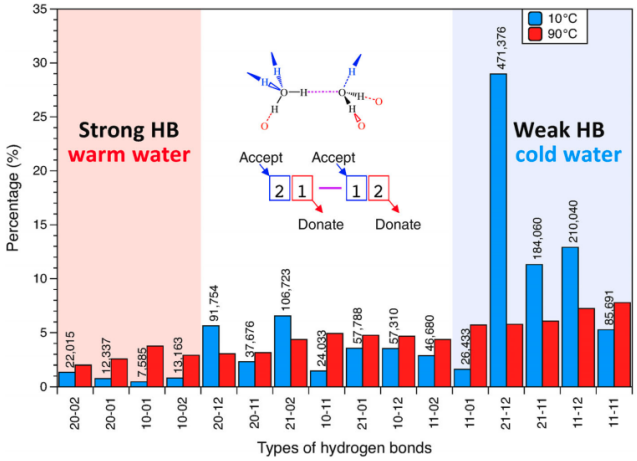
# Local Vibrational Mode Analysis




Local mode analysis of the hydrogen bonds can explain the Mpemba effect in water (warm water freezes faster than cold water).

Harmonic frequency calculations and normal mode analysis are standard in modern quantum chemistry research. However, normal modes are usually delocalized, which limits their utility in studying individual chemical bonds. In order to gain insight on local chemical bonds, Prof. E. Kraka's group has developed a software package LMODEA based on the local vibrational mode theory (see *WIREs: Comput. Mol. Sci.*, e1480 (2020)).

- Local modes are derived from normal modes via mass-decoupled Euler-Lagrange equations. Only the information about force constants and normal modes is needed.
- The LMODEA package can be easily connected to Q-Chem. After a standard Q-Chem frequency calculation, the generated .fchk file can be read by LMODEA for local mode analysis.
- Applications of local mode analysis include characterizing covalent bonds, hydrogen bonds, and weak interactions, assigning aromaticity indices, studying chemical similarity, calculation of pKa, and chiral discrimination.




Frequencies of different types of H-bonds found in the MD simulations of $(H_2O)_{1000}$ based on local mode analysis.

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