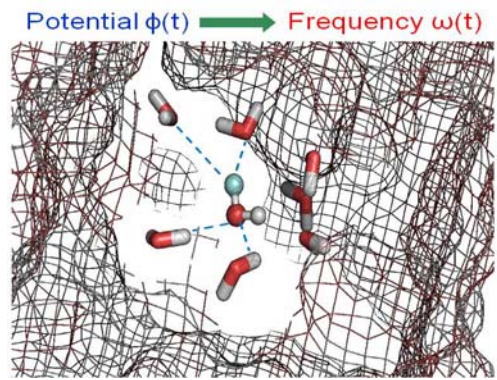


Calculation of vibrational spectrum in liquid water

Jun-Ho Choi^{a)*} and Minhaeng Cho^{a)}

^{a)}Center for Molecular Spectroscopy and Dynamics,
Institute for Basic Science, Korea University, Seoul
136-713, Republic of Korea

Keywords: MD simulation, vibrational spectrum, QM
calculation, time correlation function



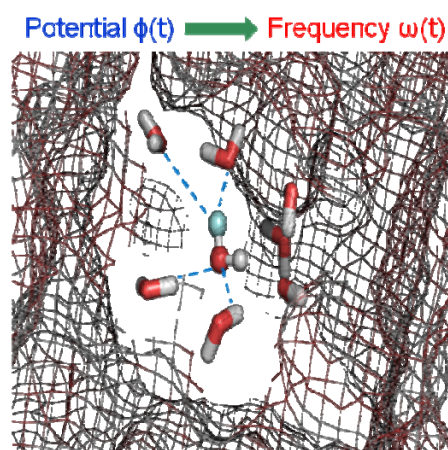
Calculation of vibrational spectrum in liquid water

Jun-Ho Choi^{a)*} and Minhaeng Cho^{a)}

^a Center for Molecular Spectroscopy and Dynamics, Institute for Basic Science, Korea University, Seoul 136-713, Republic of Korea
E-mail: jhchoi54@hanmail.net

Quantum mechanical (QM) calculation has been widely used for description of vibrational spectrum for a given molecular system by calculating transition frequency and transition dipole moment of corresponding vibrational mode. The molecule dissolved in liquid water forms hydrogen bonding with surrounding water molecules and the configuration of solute-water molecules is constantly changed causing fluctuating solvatochromic frequency and transition dipole of a given vibrational mode. Therefore, to numerically simulate vibrational spectrum in liquid water, vibrational properties need to be calculated for numerous solute-water configurations obtained from MD simulation. However, it is not practical to deal with entire solvent-solute system due to expensive computational cost of QM calculation.

We have developed a systematic theoretical way to numerically simulate vibrational spectrum in aqueous solution and showed that this approach was successfully applied to describe linear and nonlinear vibrational spectrum of amide I mode, various IR probes such as -CN, -SCN, -N₃, CO (MbCO) stretch modes.[1-3] Here, the solvent induced frequency shift was calculated by employing the equation with properly determined fitting coefficient. [1] Furthermore, OH and OD vibrational spectrum in liquid water was numerically simulated estimating time varying transition dipole moment as well as transition frequency and directly compared to experimentally measured vibrational spectrum.[4,5]



- [1] J. Jeon, S. Yang, J.-H. Choi, M. Cho, *Acc. Chem. Res.*, **42**, 1280 (2009).
- [2] J.-H. Choi, D. Raleigh, M. Cho, *J. Phys. Chem. Lett.* **2**, 2158 (2011).
- [3] J.-H. Choi, K.-W. Kwak, M. Cho, *J. Phys. Chem. B.* **117**, 15462 (2013).
- [4] J.-H. Choi, M. Cho, *J. Chem. Phys.* **138**, 174108 (2013).
- [5] J.-H. Choi, H. Kim, S. Kim, S. Lim, B. Chon, M. Cho, *J. Chem. Phys.* **142**, 204102 (2015).