dielectric spectroscopy of water and NaCl solutions: Experiments versus simulations
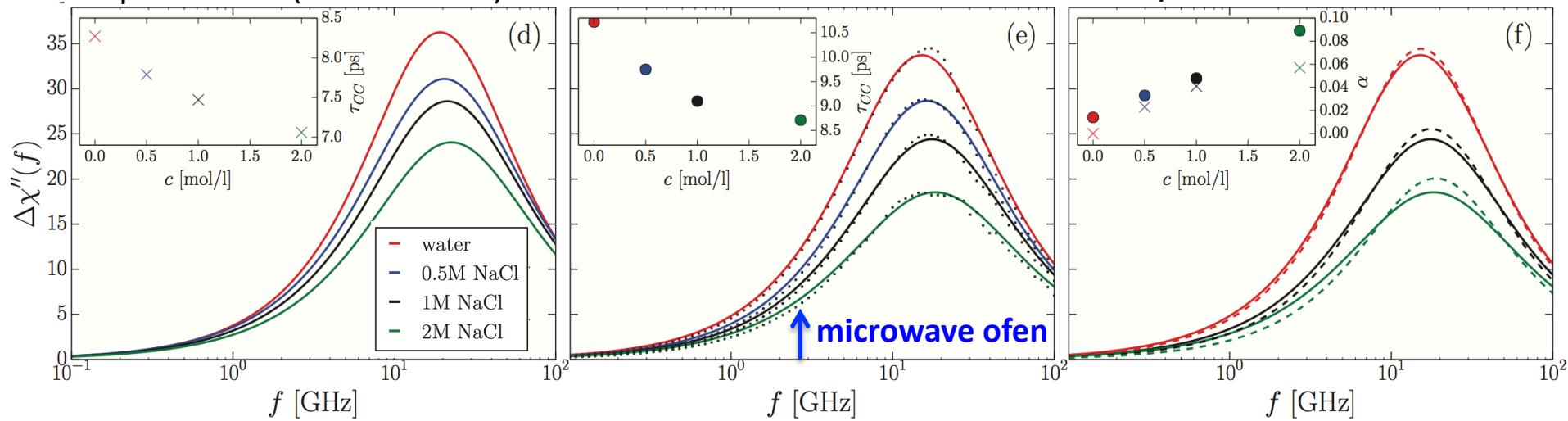
experiments (Buchner lab)

simulations

microwave ofen

Debye versus Cole-Cole fits

K. Rinne, S. Gekle, R. Netz, J. Chem. Phys. 141, 214502 (2014)
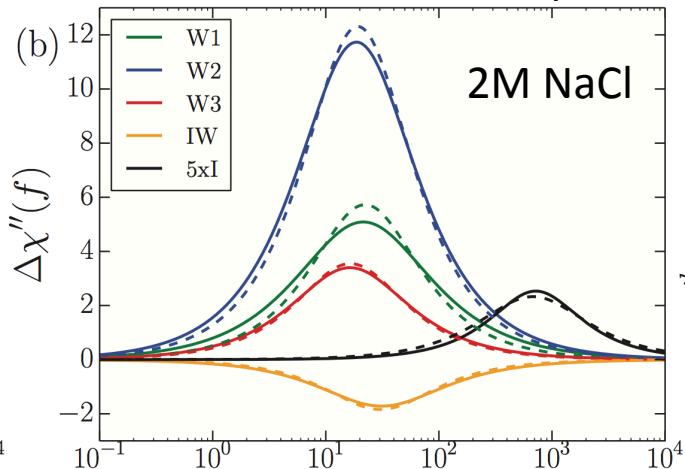
linear-response relation

$$\vec{P}(f) = \chi(f)\epsilon_0 \vec{E}(f)$$

$$\chi(f) = \chi'(f) - i\chi''(f)$$

decomposition into ionic, water and water-ionic parts

2M NaCl

FDT relation:

$$\chi(f) = -\frac{1}{3Vk_BT\epsilon_0} \int_0^\infty e^{-2\pi i f t} \langle \vec{P}(0)\dot{\vec{P}}(t)\rangle \mathrm{d}t$$

Cole-Cole fit form:

$$\Delta\chi(f) + 1 = \frac{\epsilon_{CC} - \epsilon_\infty}{1 + (i\,2\pi f \tau_{CC})^{1-\alpha}} + \epsilon_\infty$$

in simulations: splitting into water and ionic contributions

$$\vec{P} = \vec{P}_\mathrm{W} + \vec{P}_\mathrm{I}$$

$$\Delta\chi(f) = \chi_\mathrm{W}(f) + \chi_\mathrm{IW}(f) + \Delta\chi_\mathrm{I}(f)$$