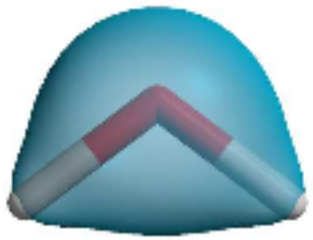
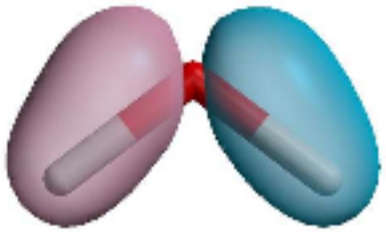
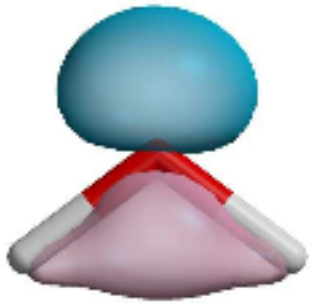
Canonical orbitals of water





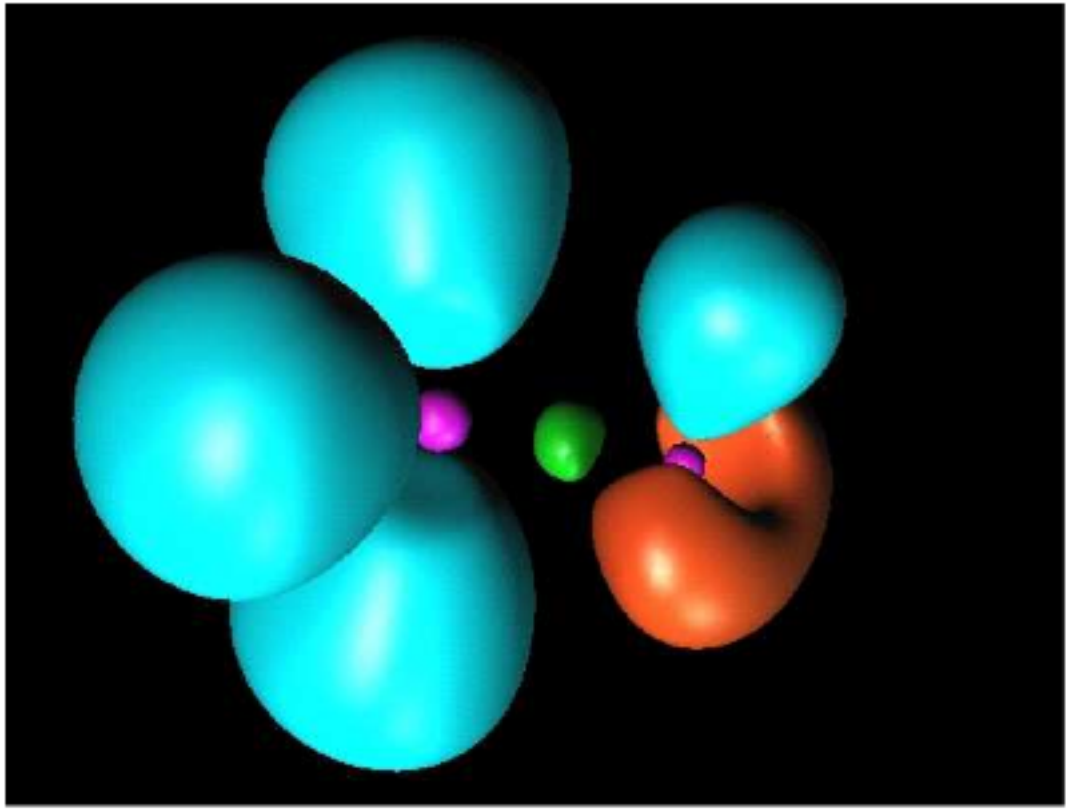


$$ELF = \left(1 + \left(\frac{d_\sigma}{d_\sigma^0}\right)\right)^{-1}$$

$$d_\sigma = \tau_\sigma - \frac{1}{4}\frac{(\nabla\rho_\sigma)^2}{\rho_\sigma} \qquad \tau_\sigma = \sum_i |\phi_i|^2 \qquad d_\sigma^0 = \frac{3}{5}(6\pi^2)^{2/3}\rho_\sigma^{5/3}$$

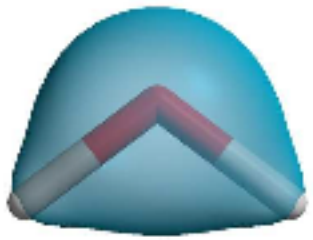
$ELF = 1$
perfect localization

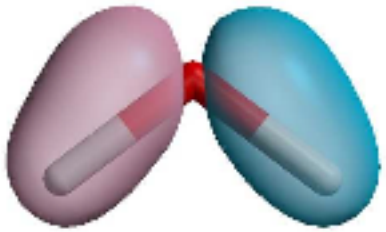
$ELF = 1/2$
Uniform electron gas

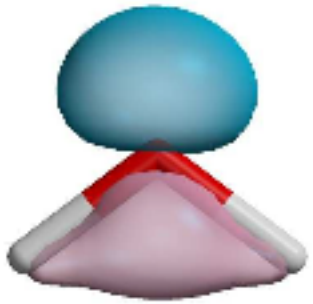


ELF of methanol

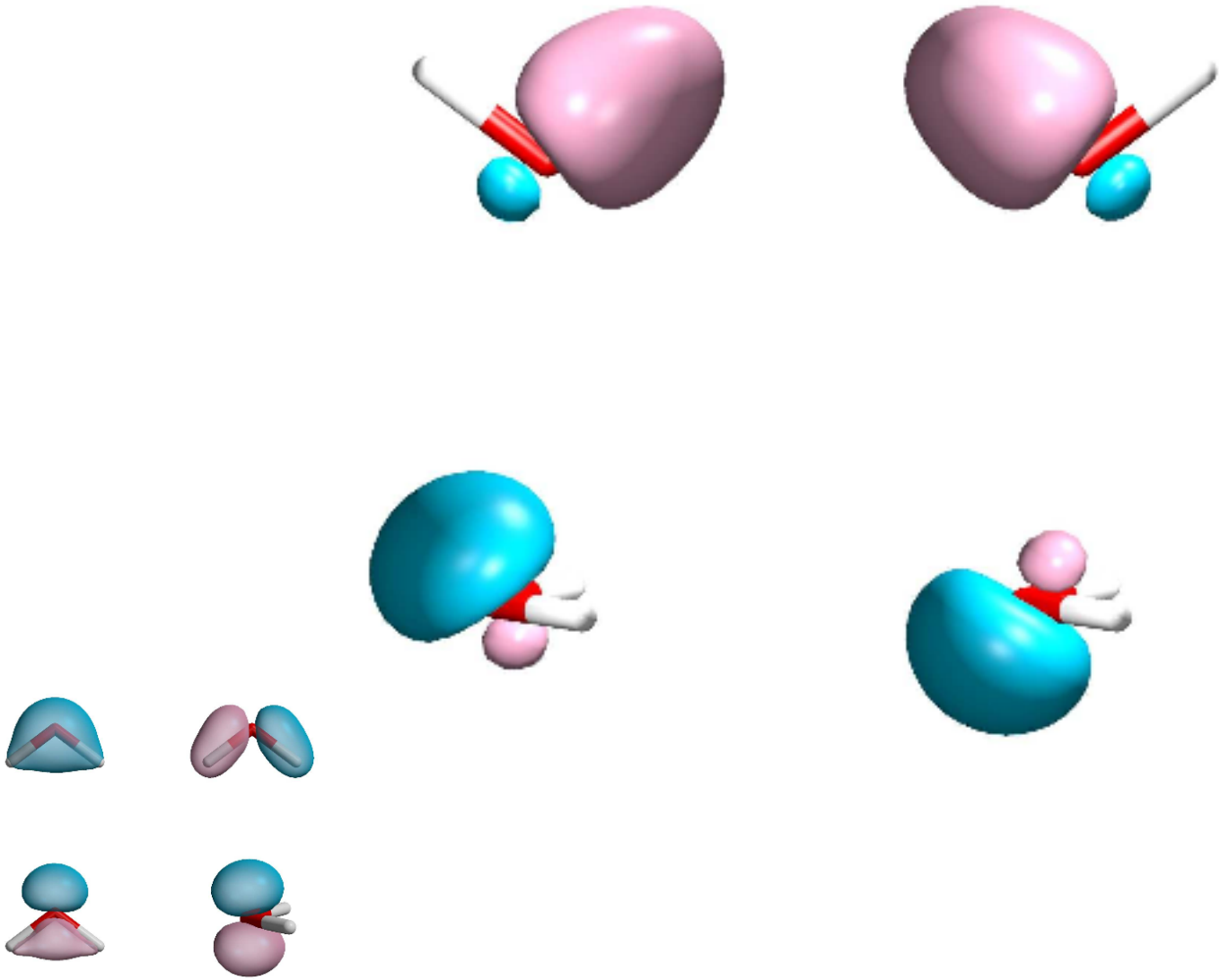
Canonical orbitals of water



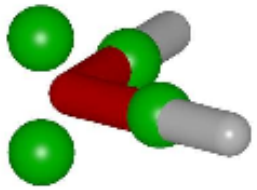




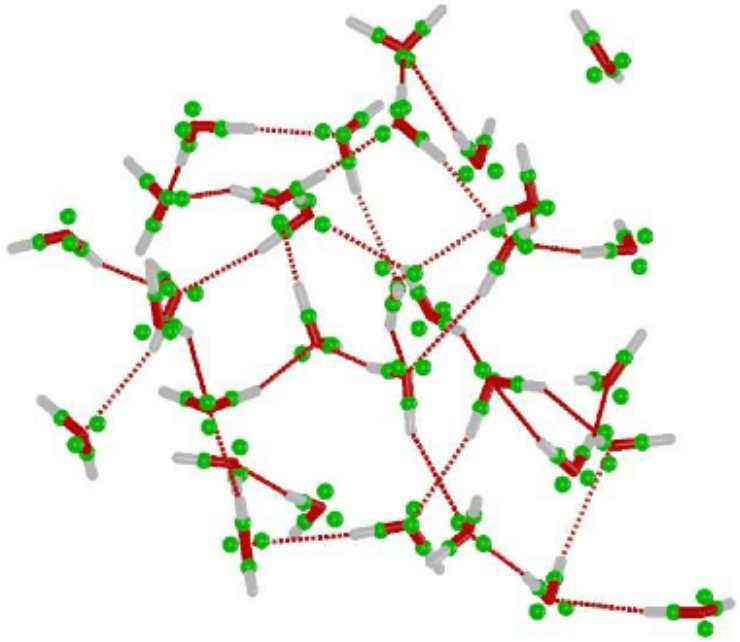
Maximally localized Wannier orbitals of water



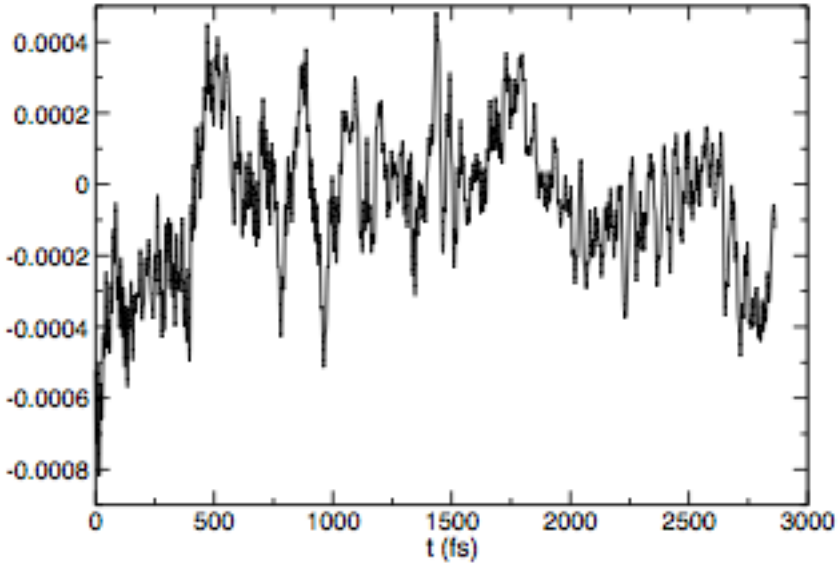
Wannier centers: isolated water

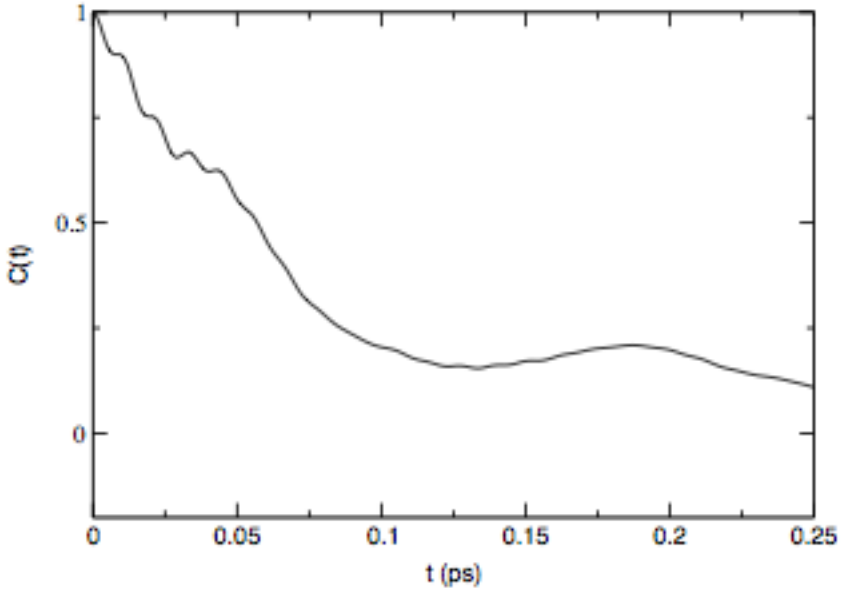


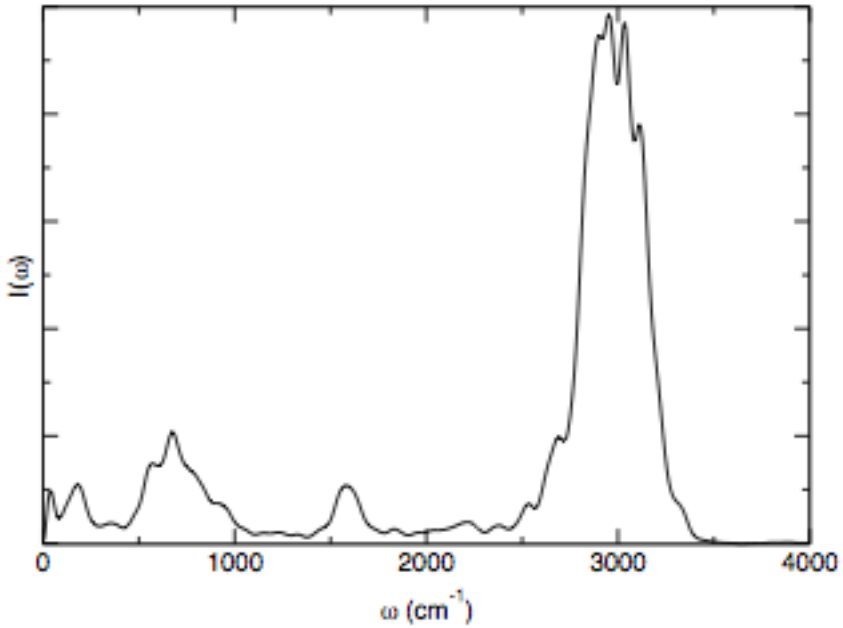
Wannier centers: liquid water



Example: infrared spectrum of water

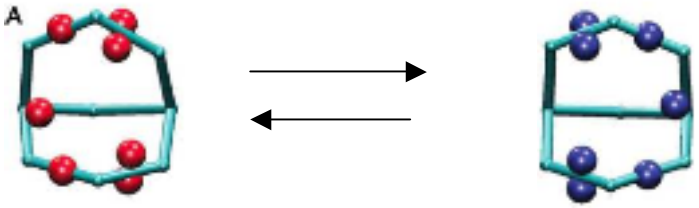




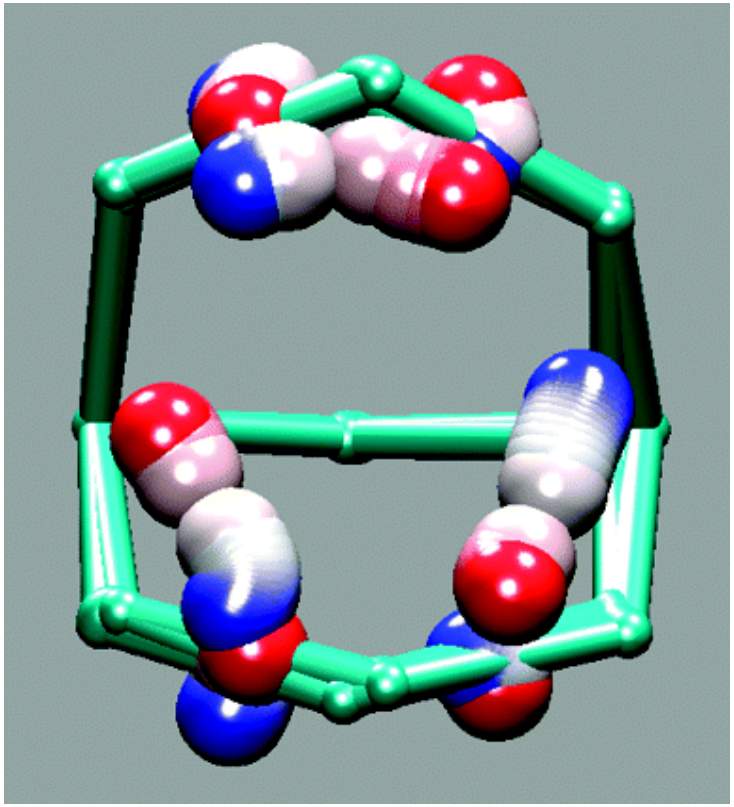


$$I(\omega) = \frac{\beta\omega^2}{2} \int_{-\infty}^{\infty} e^{i\omega t} \langle M(0)M(t)\rangle_0 dt$$

Reactivity: barbaralane isomerization



Reactivity: barbaralane isomerization



Seminal papers:

Wannier, Phys. Rev. 1937,**52**,191

N. Marzari and D. Vanderbilt, Phys. Rev. B, 1997, **56**, 12847
R. Resta, Phys. Rev. Lett. 1999, **82**, 370

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N. Marzari, I. Souza and D. Vanderbilt, *Psi-K Scientific Highlight of the Month*, No. 57 (2003)
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Rozgonyi et al. J.Phys. Chem. A, 2010, **114**,1207(barbaralane isomerization)
Zipoli et al. ChemPhysChem 2005, **6**, 1772 (Lewis-Acid- Catalyzed Hydrosilylation of Alkynes)