Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

H-bonding network and the far Infrared spectrum of liquid water[1]

MANU SHARMA, Department of Chemistry, Washington Road, Princeton University, Princeton, NJ 08544, RAFFAELE RESTA, INFM DEMOCRITOS National Simulation Center, via Beirut 2, I-34014 Trieste, Italy, ROBERTO CAR, Department of Chemistry, Washington Road, Princeton University, Princeton, NJ 08544

— We have performed Car-Parrinello molecular dynamics simulation based on maximally localized Wannier functions on a computational sample of liquid water containing 64 molecules in a cubic supercell. Using the Wannier function centers along the molecular dynamics trajectory, we have calculated the Infrared spectrum of liquid water and analyzed in detail the far Infrared region of the spectrum. We have devised several correlation functions that allow us to "cleanly" isolate the features of the spectrum in the far Infrared region. We observe that the $\sim$200 cm^{-1} peak in the Infrared spectrum arises due to dynamical charge transfer between a water molecule and its nearest neighbors. Furthermore, we provide evidence that this peak is strongly anisotropic in nature and is Infrared active only when the local H-bonding environment in liquid water changes asymmetrically.

[1] Work partially supported by the Office of Naval Research through grants N00014-01-1061, N00014-01-1047, N00014-03-0570

Manu Sharma
Department of Chemistry, Washington Road, Princeton University
Princeton, NJ 08544

Date submitted: 06 Dec 2004

Electronic form version 1.4