

MAR05-2004-004766

Abstract for an Invited Paper  
for the MAR05 Meeting of  
the American Physical Society

**Ab-initio simulations of liquid water: dielectric and hydrophobic effects<sup>1</sup>**

ROBERTO CAR, Princeton University

Hydrogen bonds are at the origin of many special properties of water. In this talk I will show how extensive *ab-initio* molecular dynamics simulations and simple theoretical models give insight on the structure and dynamics of the H-bond network. I will discuss in particular: (a) a study of the dielectric properties of water, based on simulations under a finite applied electric field, and (b) a study of the molecular origin of the hydrophobic effect, based on simulations of a solvated methane pair.

<sup>1</sup>Work partially supported by NSF through grant ITR-CHE-012432, by ONR through grant N00014-01-1-1061, and by NASA-BIMAT through grant NCC 1-02037