

Il centro NAST e il Dipartimento di Fisica  
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## **Seminario**

# **Prof. Roberto Car**

Princeton University, Princeton, New Jersey, USA

***Water at extreme conditions: from deep  
undercooling to ultrahigh pressure***

## **Aula Grassano**

Dipartimento di Fisica, Università' degli Studi di  
Roma "Tor Vergata"

**Ore 12.00 – 16 Luglio 2014**

# Water at extreme conditions: from deep undercooling to ultrahigh pressure

**Prof Roberto Car**

Princeton University, Princeton, New Jersey, USA

Structure and dynamics of water change dramatically with thermodynamic conditions. Here I will discuss computer simulations of two widely different regimes: (i) deep undercooling under moderate pressure, (ii) ultrahigh pressure under hot conditions. The phase diagram of water, at deeply undercooled conditions, may explain the origin of its thermodynamic anomalies but accessing this regime is very challenging for both experiment and simulations. The latter are currently only possible using model empirical potential interactions. Ab-initio simulations based on electronic density functional theory will be used instead to predict the behavior of water at extreme pressures and temperatures. In this regime, ionic bonding and new states of matter emerge with implications for planetary science.