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Hamburg Photon Science Colloquium –Water: from ab-initio simulations to coarse grained models

Friday 3 June 2016 14:00 (1h 30m)

The unusual properties of water, including the thermodynamic anomalies of the liquid, the existence of more than one amorphous ice form, and the abnormal mobilities of the water ions, derive from the tetrahedral network of hydrogen bonds that hold the molecules together. Modern ab-initio simulations had to overcome major challenges to successfully predict the properties of ambient water from the basic molecular interactions and dynamics. These studies reveal features of the coupled dynamics of electrons and nuclei that would not be otherwise accessible.

Understanding the microscopic origin of the thermodynamic anomalies of liquid water has been a long-standing issue in this field. The behavior of metastable water at deeply undercooled conditions may hold the clue for resolving this issue. The very long time scales associated with the relaxation processes of the hydrogen bond network at undercooled conditions make these studies only feasible with coarse-grained models. Recent progress in this context will be presented.

The connections of theory, simulation, and experiment will be stressed throughout the lecture.

Presenter: Prof. CAR, Roberto (Princeton University)