

## Structure and dynamics in cold aqueous clusters: quantum and classical perspectives



## Prof. Peter J. Rossky

Department of Chemistry, Rice University, Houston, Texas

Date & Time: 2017/3/13 (Mon.) 17:00-17:55 Place: IMS Research Building Room 201

In this presentation, the results of a number of theoretical studies focusing on the dynamics and distribution of hydrogen atoms in cold charged and neutral water clusters will be discussed. The role of low temperature in the creation of nonequilibrium states will be considered, as will the important role of such cold conditions in amplifying the importance of quantum isotope effects. The potential use of the latter effects as an indirect experimental signature of the internal thermal state of clusters will be discussed.



Contact : Shinji Saito (Theoretical and Computational Molecular Science) Ryota lino & Takeshi Yanai (IMS colloquium FY2016 committee)