



# IRTG-Seminar

## Prof. Dr. Yunjie Xu

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### **“An unusual water tunneling path in the methyl glycidate-water complex and solvation of methyl glycidate in water”**

Methyl glycidate is a chiral epoxy ester whose structure and characteristic functional groups can be used to model biological events involving much larger chiral esters on the molecular scale. In this presentation, I will discuss rotational spectra of methyl glycidate monohydrate and some interesting splitting observed. In particular, an unusual water tunneling path was proposed for this tightly bound system to explain the relatively large splitting measured. In addition, I will show vibrational circular dichroism and Raman optical activity spectra of methyl glycidate in  $\text{CCl}_4$  and water. The link between the small methyl glycidate hydrates and the main long-lived species which exist in aqueous solution is emphasized in the context of the clusters-in-a-liquid solvation model.

**Tuesday, August 22, 2017, 9:00 a.m.,  
5<sup>th</sup> floor, Seminar room,  
Physics high-rise, Hermann-Herder-Str. 3**