

# SEMINAR ANNOUNCEMENT

Friday, 16.01.2015 | 14 h c.t. | NC 6/99

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## "Dissecting solvent-solvent and solvent-solute interactions step by step: The case of methanol"

### Abstract:

Structurally simpler than liquid water and equipped with the possibility of chemical variation, methanol is an interesting protic solvent. We try to contribute to a fundamental understanding of this solvent by applying linear vibrational spectroscopy tools to its isolated clusters. Already the dimer of methanol poses some challenges which are only partially understood. How anharmonic is the OH bond when it engages in a hydrogen bond <sup>[1]</sup>? Which fraction of the hydrogen bond-induced OH stretching shift is harmonic in origin <sup>[2]</sup>? Why do DFT methods and also MP2 fail in quantitatively describing this shift? How anharmonic is the librational motion of the OH group orthogonal to the hydrogen bond? What happens if we mix other solvent molecules, such as acetone <sup>[3]</sup>, or an alkene, or diphenylether, with methanol? The talk will cover some of these questions and our proposed answers.

- [1] F. Kollipost, K. Papendorf, Y.-F. Lee, Y.-P. Lee, M. A. Suhm, Alcohol dimers - how much diagonal OH anharmonicity?, *Phys. Chem. Chem. Phys.* **16** (2014) 15948-15956
- [2] M. Heger, M. A. Suhm, R. A. Mata, Communication: Towards the binding energy and vibrational red shift of the simplest organic hydrogen bond: Harmonic constraints for methanol dimer, *J. Chem. Phys.* **141** (2014) 101105
- [3] F. Kollipost, A. Domanskaya, M. A. Suhm, Microscopic Roots of Alcohol-Ketone Demixing: Infrared Spectroscopy of Methanol-Acetone Clusters, *J. Phys. Chem. A* (2014), in press