

# IRTG-Seminar

## Prof. Peter Hamm

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### “2D-IR Spectroscopy at its Best: Structure and Dynamics of Catalytic Molecules at Solid/Liquid Surfaces”

2D-IR spectroscopy can tell us a lot about solvation dynamics, structural dynamics and energy transfer processes of molecular systems in different environments. After an introduction into the concepts of multidimensional spectroscopy, I will illustrate its capability by discussing structure and dynamics of molecules immobilized at solid/liquid surfaces, which play an important role in electro- and photocatalysis. For example, time-dependent inter-molecular cross peaks between two isotopomers of a CO<sub>2</sub>-reduction catalyst originate from through-space transition-dipole coupling (Fig. 1). From the transfer rate, we can estimate that the molecules are bound to the surface with essentially a closest packing. With the help of the solvent, the morphology of the monolayer can be controlled, inducing partial order. We furthermore studied the vibrational energy transfer rate on different types of surfaces with different levels of plasmonic enhancement, and somewhat surprisingly find that the transfer rate is not affected, an effect that is explained with the help of an image-dipole picture. Finally, the 2D IR spectroscopy of the Pt-H bond will be discussed, a transient species which must appear during electrolysis with Pt still being the only water-splitting catalyst that is of technological relevance.

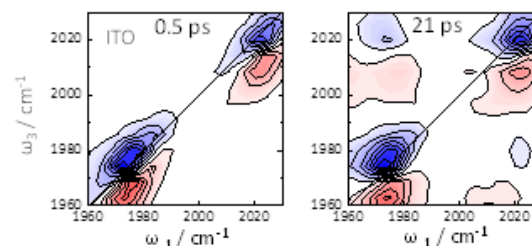


Figure 1: 2D ATR IR spectrum of [Re\(4,4-dicarboxyl-2,2-bipyridine\)\(13/12CO\)<sub>3</sub>Cl/Br](#) on an ITO surface. Cross-peaks appear as a function of population time.

**Tuesday, January 16, 2018, 1:00 p.m., HS II,  
Physics high rise, Hermann-Herder-Str. 3**