Revealing Reaction Mechanisms Using Raman Spec and Quantum Chemistry

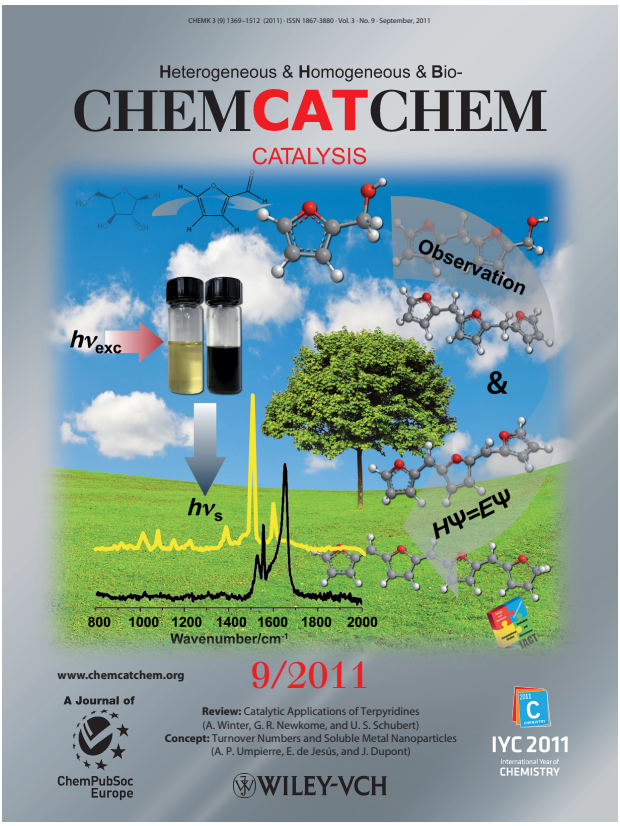
Vibrational methods are one of the most powerful spectroscopic techniques used to understand the nature of reactants, products, and intermediates. One popular method, Raman spectroscopy, provides molecular insight into the catalytic reaction and the nature of intermediates. Density functional methods provide molecular structure details for reactants, products, and intermediates; provide detailed energetics of the reaction profile; and also predict vibrational spectra of intermediates with minimal computational demand compared to high-level methods.

The Challenge

To confirm controversial intermediate species (dienes and diketones) and reaction mechanisms of furfuryl alcohol polymerization. This chemical is derived from biomass and is a sustainable building block for polymeric materials and alternative fuels.

The Solution

Using Raman spectroscopy and density functional methods, an experimental and theoretical research team led by Christopher Marshall identified the molecular intermediates and reaction mechanisms during the polymerization of furfuryl alcohol.



The cover picture shows furfuryl alcohol polymerization, an important reaction during the mineral acid treatment in aqueous solution.

The Results

A strong aliphatic C=C band observed in both the calculated and measured Raman spectra provides crucial evidence for understanding the furfuryl alcohol polymerization reaction. The team confirmed that the formation of a conjugated diene structure, rather than a diketone structure, is involved in the polymerization reaction.

"By combining experimental and theoretical investigations, we can provide a more detailed molecular understanding of polymerization during the conversion of biomass to alternative fuels and industrial chemicals," **said chemist Christopher Marshall.**

For further information, contact: Christopher Marshall, marshall@anl.gov

March 2012