

# Investigating Molecular Structures



Jochen Autschbach

Assistant Professor, Department of Chemistry Associate Professor, Chemistry Full Professor,  
Department of Chemistry

## CURRENT RESEARCH

Using theoretical chemistry to investigate molecular structures and chemical bonding, and how they relate to the desired functionality of a synthesized molecule

Theoretical chemistry is playing an increasingly crucial role in the development of new drugs, new chemical catalysts, and new molecular materials. Theory can even predict new molecules with desired properties that ought to be synthesized. Dr. Jochen Autschbach uses theory and computer simulations to understand how molecular structures (the 'shapes' of a molecule) and chemical bonding determine what can be observed in the laboratory for a variety of chemical compounds. When data is limited or experimentation is very difficult - as it often is - theory provides an ideal alternative way for gaining insight into new compounds. Dr. Autschbach's research focuses on how the basics of chemistry connect to later discovery and outcomes. It strengthens the scientific software infrastructure and contributes to society by identifying and improving chemical catalysts used to make plastics and other types of polymer materials, by joining efforts with nuclear waste clean-up, and by identifying potentially harmful molecular variants of drug molecule candidates.

Dr. Jochen Autschbach, Professor in the Department of Chemistry at the University of Buffalo, State University of New York, is working with quantum theory, which predicts accurately what electrons and atomic nuclei do in molecules. He is predicting optical and 'spectroscopic' properties of molecules and molecular materials, and understanding how these properties relate to molecular structures and chemical bonding. This data is critical for the rational design of new molecules and, for existing compounds, to know why laboratory observations return the results that they do. In spectroscopy, electric or magnetic fields of varying frequency are used for...

## AFFILIATION



University at Buffalo, SUNY

## EDUCATION

- Ph.D., in Theoretical Chemistry, 1999 , University of Siegen, Germany
- Diploma, in Chemistry, 1996 , University of Siegen, Germany

## AWARDS

- NSF CAREER Award, 2005
- UB Exceptional Scholar Award (Young Investigator), 2007

## RESEARCH AREAS

Technology, Chemistry

## FUNDING REQUEST

Your contributions will support talented members of Dr. Autschbach's team: post-doctoral researchers with experience in scientific programming for developing new simulation methods, summer stipends to supplement teaching assistant stipends for graduate students, and summer stipends for undergraduate students to have their first hands-on research experience. Contributions will also allow for the updating and replacing of computer equipment to ensure competitiveness in the field.

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