

# Shane M. Parker



**Graduate Institution:** Northwestern University

**Graduate Discipline:** Theoretical Chemistry

**Hometown:** Punta Gorda, FL

**Relevant SC Research:** Basic Energy Sciences

## Research Interest:

My current interest is in simulating control the internal motions of molecules (for example, torsion in biphenyl) using coherent laser pulses. Torsion in biphenyl can determine the extent of electronic coupling between the two phenyl rings, thus controlling properties such as the absorption and fluorescence spectra and electron transfer and transport rates. Since biphenyl exhibits axial chirality, torsion also converts between enantiomers

We have shown via simulation that short moderately intense lasers pulses can initiate torsion or select between enantiomers a pre-oriented thermal ensemble of biphenyl derivatives in the gas phase.

We are currently working to extend that motif to control a molecule adsorbed to a surface. Recent experiments have shown that chiral thin films can act as spin-filters for spin-polarized electrons. Thus, controlling torsion of a molecular thin film can control both the electron transfer rates as well as the spin-filter properties of the thin film.

I am also interested in using wavefunction based electronic structure methods to study exciton fission in organic crystals.

## About Me:

My interest in theoretical chemistry was born while studying quantum mechanics with Yngve Öhrn as an undergraduate chemistry and mathematics major at the University of Florida. After graduating in 2008, I spent a year with Professor Notker Rösch at the Catalysis Research Center of the Technical University of Munich as a Fulbright Fellow, researching in catalysis, practicing my German, and enjoying lovely Munich, Germany, and Europe. One of the highlights from that year was the opportunity to attend the Lindau meeting of the Nobel laureates in Lindau, Germany. Since September 2009 I have been a graduate student at Northwestern University, joint between Professors Tamar Seideman and Mark Ratner.

When I am not thinking about chemistry, I can often be found holding a camera in front of my face or rock climbing, both interests I picked up from my brother. I also thoroughly enjoy cooking, traveling, attempting to learn new languages, and sharing those experiences with friends.



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