David Stuck

Graduate Institution: University of California - Berkeley

Graduate Discipline: Theoretical Chemistry

Hometown: Valparaiso, IN

Relevant SC Research: Basic Energy Sciences

Research Interest:

My primary research interests lie in developing methods to study the electronic structure of molecules for which standard mean field theory does not give the best approximate orbitals. This important class of systems includes many open shell molecules, which are characterized by spin-contaminated mean field wave functions that typically perform poorly as the basis for higher-level theories. Accurately calculating the properties of chemicals that suffer from spin-contamination is important particularly in studying catalytic cycles involving changes in spin state and for probing reaction mechanisms with single bond dissociations.

Another recent interest is in using path integral quantum mechanics to extend the applicability of electronic structure theory. Path integral methods give a practical way to apply quantum mechanics to nuclear coordinates to calculate properties such as the zero point energy or dynamics that involve a coupling of electronic and nuclear degrees of freedom.

About Me:

I am currently beginning my third year studying electronic structure theory under Martin Head-Gordon at UC, Berkeley. Previously, I studied chemistry and mathematics at Trinity University in San Antonio, TX where I worked for two years in a physical organic chemistry lab doing synthetic chemistry before being introduced to the world of quantum chemistry in my final year. I traded stinking organics and noxious acids for white boards and computers and don't plan on going back.

My goal has always been to be a research scientist, but my experience as a graduate student instructor for introductory quantum mechanics has reinforced my desire for teaching to also be a part of my career. To this end, I currently plan to pursue a post-doc and then a professorship.

Although I miss the heat of San Antonio, I enjoy exploring all the nature, food, and culture the Bay Area has to offer with my wife and friends. Additionally, I like to spend my free time cooking, getting beat at chess, and watching good movies.