Curriculum Vitae

Andrew Powell

Missouri University of Science and Technology
142 Schrenk Hall, Department of Chemistry
400 West 11th Street
Rolla, MO 65409-0010
Mobile Phone: (816) 520-1175
adpkd6@mst.edu

Education:

Ph. D., Chemistry -- Missouri University of Science and Technology. 2012-2017 (Expected).

- Quantum Monte Carlo for Reaction Dynamics (Dr. Richard Dawes)

B.S., Chemistry and Mathematics -- College of the Ozarks. 2007-2011.

Publications

1. Aimable Kalume, Lisa George, Andrew D. Powell, Richard Dawes and Scott A. Reid, Photoinduced Electron Transfer in Donor–Acceptor Complexes of Ethylene with Molecular and Atomic Iodine, *J. Phys. Chem. A* **118**, 6838 (2014).

2. Andrew D. Powell and Richard Dawes, Calculating Potential Energy Curves with Fixed-Node Diffusion Monte Carlo: CO and N_2, *J. Chem. Phys*. **145**, 224308 (2016).

In Preparation

1. Investigation of the Ground State Reaction Pathway for $O + O_2 \rightarrow O_3$ with Full Configuration Interaction Quantum Monte Carlo and Fixed-Node Diffusion Monte Carlo, A Comparison with Contracted and Uncontracted MRCI, Andrew D. Powell and Richard Dawes.

2. Investigation of Reaction Barriers that are Sensitive to Dynamic Electron Correlation Using Fixed-Node Diffusion Monte Carlo, Andrew D. Powell and Richard Dawes.

Conference Presentations and Posters

“Using Specific Conductivity of Dilute Nitrate Salts to Demonstrate Periodicity.” American Chemical Society National Meeting & Exposition, Anaheim, CA, March 27-31, 2011. (Poster)

“Using Specific Conductivity of Dilute Nitrate Salts to Demonstrate Periodicity.” Missouri Academy of Science, Jefferson City, MO, April 2011. (Presentation)

"Calculating Potential Energy Curves with Quantum Monte Carlo." 69th International Symposium for Molecular Spectroscopy, Urbania-Champaign, IL, June 16-20 2014. (Presentation)

"Calculating Potential Energy Curves with Quantum Monte Carlo." Mid-West Regional ACS Meeting, Columbia, MO, November, 12, 2014. (Poster)

"Applying Quantum Monte Carlo to the Electronic Structure Problem." 71st International Symposium for Molecular Spectroscopy, Urbania-Champaign, IL, June 20-24 2016. (Presentation)

Professional Memberships and Associations

Sigma Zeta, Member (2010-present)

American Chemical Society

Skills

Quantum Chemistry Codes

- MOLPRO, GAMESS, GAUSSIAN

Quantum Monte Carlo Codes

- CASINO, NECI, QMCPACK

Programming

- Fortran, Matlab, scripting and data processing

Languages

English (Native)

References

Dr. Richard Dawes
Associate Professor
Chemistry
142 Schrenk Hall
Rolla, MO 65409
(573) 341-4451
dawesr@mst.edu

Dr. Jeffrey Winiarz
Associate Professor
Chemistry
332 Schrenk Hall
Rolla, MO 65409
(573) 341-6733
winiarzj@mst.edu

Dr. Albert Dixon
Associate Professor
Mathematics-Physics
216 Pfeiffer Building
Point Lookout, MO 65726
(417) 690-3379
dixon@cofo.edu