Scott Yockel

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Education

Postdoctoral Research, September 2006-present, University of North Texas, Denton, Texas
Advisor: Paul S. Bagus

Ph.D. Chemistry, August 2006, University of North Texas, Denton, Texas
Dissertation: “The evaluation, development, and application of the correlation consistent basis sets”
Advisor: Angela K. Wilson

B.S. Chemistry, May 2000, Oklahoma Baptist University, Shawnee, Oklahoma

Honors and Awards

NSF Panelist Invitation for Korean-American Scientist and Engineers Association Annual Meeting, 2006
NSF East Asia and Pacific Summer Institutes (EAPSI) Graduate Fellowship, 2005
ACS Division of Computers in Chemistry, Chemical Computing Group (CCG) Excellence Award, 2005
B. Craig Raupe Memorial Scholarship, 2003, 2004, 2005, 2006
Robert B. Toulouse School of Graduate Studies Travel Grant, 2001, 2005
James J. and Ruth I. Spurlock Scholarship Award, 2006

Professional Training

American Chemical Society Petroleum Research Fund - Summer School: "Time-Dependent Density Functional Theory and the Dynamics of Complex Systems." St. John's College, Santa Fe, New Mexico, June 2004

Employment

University of North Texas, Denton, Texas
Postdoctoral Research Associate with Paul S. Bagus. September 2006-present
Research Assistant for Professor Angela K. Wilson. Physical and Theoretical Chemistry. 2003-2006
Teaching Assistant for Professor Angela K. Wilson. Computational Chemistry. 2003-2004
Teaching Assistant for Professor Paul Jones. Organic Chemistry. 2002-2003
Teaching Assistant for Professor Jim Marshall. General Chemistry. 2001-2002

Pohang University of Science and Technology, Pohang, South Korea
Research Assistant for Professor Kwang S. Kim at Center for Superfunctional Materials. 2005

Southwell Laboratory, Inc., Oklahoma City, Oklahoma
Chemical Analyst, Organic Chemistry Department, 2000-2001

Skills

Computer system administration, with six years experience (1) building complete computing systems/clusters from ground up (installing hardware, operating systems, RAID devices, compilers, batch queuing systems, compiling scientific software codes) for various UNIX (Irix, Solaris, HP-UX) and Linux (OS X, Enterprise, Fedora, Debian) based systems, (2) configuring parallel computing interfaces: MPI, GA, GM (Myrinet) and network file systems (3) managing user accounts, queuing systems, and security/firewall.

Proficient with python, awk, and other scripting languages/tools and limited experience with Fortran and C.

Extensive experience with software codes MOLPRO, Gaussian, Alchemy, Molden and proficient with GAMESS, Dirac, Turbomole, Spartan.

Professional Societies

Member of the American Chemical Society, 2002-present

Publications

S. Yockel and A. K. Wilson, “Erratum to ‘SO3 revisited: Impact of tight d augmented correlation consistent basis sets on atomization energy and structure’ [R. D. Bell and A. K. Wilson, Chem. Phys. Lett. 394 (2004) 105109]” *Chem. Phys. Lett.* **394,** 105 (2006).

N. J. DeYonker, T. Grimes, S. Yockel, A. A. Dinescu, B. Mintz, A. K. Wilson, and T. R. Cundari, “Modifications to the Correlation Consistent Composite Approach (ccCA) and Benchmarking with the G3/99 Test Set.” *J. Chem. Phys.* **125,** 104111 (2006).

S. Yockel, A. Garg, and A. K. Wilson, "The Existence of $FKrCF_3$, $FKrSiF_3$, and $FKrGeF_3$: A Theoretical Study." *Chem. Phys. Lett.*, **411**, 91 (2005)

S. Yockel and A. K. Wilson, "Relativistic Effect Using Douglas-Kroll Contracted Basis Sets and Correlation Consistent Basis Sets with Small-Core Relativistic Pseudopotentials." *J. Chem. Phys.*, **122**, 174310 (2005)

S. Yockel, B. J. Mintz, and A. K. Wilson, "Accurate Energetics of Small Molecules Containing Third Row Atoms Ga-Kr: A Comparison of Advanced Ab Initio Methods and Density Functional Theory." *J. Chem. Phys.*, **121**, 60 (2004)

S. Yockel, J. J. Seals III, and A. K. Wilson, "An Ab Initio Study of the Noble Gas Compound HKrCl." *Chem. Phys. Lett.*, **393**, 448 (2004)

The following submitted manuscripts are in draft form, and are available upon request:

A. Lewera, W. P. Zhou, R. Hunger, W. Jaegermann, A. Wieckowski, S. Yockel and Paul S. Bagus. "The Paradox of Core-level Binding Energy Shifts in Pt-Ru Nanoparticles." *Submitted to Chemical Physics Letters.*

S. Yockel, A. K. Wilson, “Core-valence Correlation Consistent Basis Sets for Second-row Atoms (Al-Ar) Revisited” *Theoretical Chemistry Accounts - accepted.*

O. El-bjeirami, S. Yockel, C. F. Campana, A. K. Wilson, M. A. Omary “Photophysics and Bonding in Neutral Gold(I) Organometallic Complexes with an Extended-Chain Supramolecular Structure” *Organometallics - accepted.*

E. Gawlik, S. Yockel, A. K. Wilson, “Insertion of Krypton into Halogenated Acetylene: A Theoretical Study.” S*ubmitted to the Journal of Physical Chemistry A.*

Presentations

“An Evaluation of Electron Affinities for Third-Row Atoms Ga-Kr.” S. Yockel, A. K. Wilson. *American Chemical Society Meeting-in-Miniature*, University of Dallas, Dallas, Texas. April 2002.

“Energetic and Structural Properties: Third-Row Atom Clusters.” S. Yockel, A. K. Wilson. *American Conference on Theoretical Chemistry*, Champion, PA. July 2002.

“A Comparison of the Performance of Density Functional Theory and Ab Initio Methodology for Third-Row Atom Clusters.” S. Yockel, Angela K. Wilson. *Southwest Regional Meeting of the American Chemical Society*, Austin, Texas. November 2002.

“Structures and Energetics of Third-Row Atom Clusters: A Comparison of Ab Initio and Density Functional Theory.” S. Yockel, B. Mintz, A. K. Wilson. *American Chemical Society National Meeting*, New Orleans, Louisiana. March 2003.

"A Theoretical Study of the Noble Gas Compounds HKrF and HKrCl." S. Yockel, J. J. Seals III, A. K. Wilson. *American Chemical Society National Meeting*, New Orleans, Louisiana. March 2003.

"Accurate Energetics of Small Third-Row Molecules: A Comparison of Ab Initio and Density Functional Theory." S. Yockel, B. Mintz, A. K. Wilson. *American Chemical Society Meeting-in-Miniature*, Texas A&M University-Commerce, Commerce, Texas. April 2003.

"Accurate Energetics of Small Molecules Containing Ga-Kr: A Comparison of CCSD(T) and B3LYP." S. Yockel, B. Mintz, A. K. Wilson. *Midwest Theoretical Chemistry Conference*, Iowa State University, Ames, Iowa. June 2003.

"Structure and Energetics of Third-Row Atom Clusters: A Comparison of Ab Initio and Density Functional Theory." S. Yockel, B. Mintz, A. K. Wilson. *International Union of Pure and Applied Chemistry Congress and Conference of The Canadian Society for Chemistry*, Ottawa, Ontario. August 2003.

"B3LYP and CCSD(T) Investigation of the Energetic and Structural Properties of Small Third-row Main Group (Ga-Kr) Molecules." S. Yockel, B. Mintz, A. K. Wilson. *Southwest Regional Meeting of the American Chemical Society*, Oklahoma City, OK. October 2003.

"A Not-so-noble Gas: The HKrCl molecule." S. Yockel, James J. Seals III, A. K. Wilson. *American Chemical Society Meeting-in-Miniature*, Texas Wesleyan University, Fort Worth, Texas. April 2004.

"Accurate Energetics and Structural Determination of Small Third-Row Molecules Involving Ga-Kr: An In-depth Study Using the Correlation Consistent Basis Sets". S. Yockel, B. Mintz, A. K. Wilson. *Southeast Theoretical Chemistry Association Meeting*, University of Mississippi, Oxford, Mississippi. May 2004.

"Accurate Energetics of Small Molecules Containing Third-Row Atoms Ga–Kr: A Comparison of CCSD(T) and B3LYP Methods." S. Yockel, Benjamin Mintz, A. K. Wilson. *American Chemical Society's Petroleum Research Fund Summer School: Time-Dependent Density-Functional Theory and the Dynamics of Complex Systems*, St. John's College, Santa Fe, New Mexico. June 2004.

"Examining the Intrinsic Error in CCSD(T) and B3LYP for Small Third-row Molecules Using the Correlation Consistent Basis Sets." S. Yockel, B. Mintz, A. K. Wilson. *Molecular Quantum Mechanics: An International Conference in Honor of Professor Nicholas C. Handy*, St. John's College, Cambridge University, England. July 2004.

"Examining Relativistic Effects on Molecular Properties of the G2 Test Suite for Third-row Systems by Using Both Douglas-Kroll and Pseudopotential Correlation Consistent Basis Sets." S. Yockel and A. K. Wilson. *Southwest Regional Meeting of the American Chemical Society*, Fort Worth, Texas. October 2004.

"Heavy Group 14 Bonding to Krypton: A Theoretical Study of the Existence of $FKrSiF_3$ and $FKrGeF_3$." A. Garg, S. Yockel, A. K. Wilson. *Southwest Regional Meeting of the American Chemical Society*, Fort Worth, Texas. October 2004.

"Theoretical Study of the Existence of $FKrCF_3$, $FKrSiF_3$, and $FKrGeF_3$." S. Yockel, A. Garg, and A. K. Wilson. *American Chemical Society National Meeting*, San Diego, California. March 2005.

"Structure-luminescence Relationship and Photochemistry of Neutral $LAu^{(I)}Cl$ Complexes (L=CO or RNC)." O. El-bjeirami, S. Yockel, A. K. Wilson, M. A. Omary. *American Chemical Society National Meeting*, San Diego, California. March 2005.

"Structures and Energetics of Small Third-row Molecules Determined with Correlation Consistent Basis Sets." S. Yockel and A. K. Wilson. *American Chemical Society National Meeting*, San Diego, California. March 2005.

"Krypton Bonding in $FKrCF_3$, $FKrSiF_3$, and FKrGeF3." S. Yockel, A. Garg, A. K. Wilson. *American Chemical Society Meeting-in-Miniature*, University of Texas at Arlington, Arlington, Texas. April 2005.

"New Krypton Bonded Molecules: A Theoretical Study." S. Yockel, A. Garg, A. K. Wilson. *American Chemical Society National Meeting*, Washington D.C., August 2005.

"Transition Metal Chemistry: Towards Accurate Energetic Description." J. Determan, S. Yockel, T. Grimes, M. A. Omary, P. S. Bagus, T. R. Cundari, A. K. Wilson. *American Chemical Society National Meeting*, Washington D.C., August 2005.

"Revisting the Core-valence Correlation Consistent Basis Sets for Second-row Atoms" S. Yockel, A. K. Wilson. *Quantitative Quantum Chemitry: An International Workshop in Honor of Professor Thom H. Dunning, Jr.* Santa Fe, New Mexico, March 2006.

"A Computational Study on the Stability of New Krypton-bonded Molecules." S. Yockel, E. Gawlik, A. K. Wilson. *American Chemical Society National Meeting*, Atlanta, Georgia, March 2006.

"The Relationship Between Structure and Luminescence of $Au^{I}(CO)Cl$" S. Yockel, O. El-Bjeirami, A. K. Wilson, M. A. Omary. *American Chemical Society National Meeting*, Atlanta, Georgia, March 2006.

"Core-valence Correlation Consistent Basis Sets Revisited for Second-row Atoms (Al-Ar)." S. Yockel, A. K. Wilson. *American Chemical Society National Meeting*, Atlanta, Georgia, March 2006.

"Re-examining the core-valence correlation consistent basis sets for second-row atoms (Al-Ar)." S. Yockel, A. K. Wilson. *American Chemical Society Meeting-in-Miniature*, Texas Womens University, Denton, Texas. April 2006.

"Reliable energetic prediction for the G3/99 test set and extended systems: The correlation-consistent Composite Approach (ccCA)." A. K. Wilson, N. DeYonker, T. R. Cundari, T. Grimes, S. Yockel, A. Dinescu, B. Mintz. *American Chemical Society National Meeting*, San Fransico, California, September 2006.

"Distance dependence of the core-level binding energy shifts in pure and mixed metal nanoparticles." P. S. Bagus and S. Yockel. *American Chemical Society National Meeting*, Chicago, Illinois, March 2007.

Invited Talks

"Exposure to Innovative Research in Computational Chemistry." S. Yockel. *NSF Panel at US-Korea Conference on Science and Engineerin*g. Teaneck, New Jersey, August 2006.

"Density Functional Theory." S. Yockel. *Center for Advanced Scienctific Computing and Modeling (CASCaM) Workshop*. University of North Texas, Denton, Texas, November 2006.

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