

Lucy W. Kiruri

CONTACT INFORMATION	Kenyatta University Chemistry Department P. O. Box 43844-00100 Nairobi, Kenya	voice: 0721 96***8 kiruri.lucy@ku.ac.ke
RESEARCH INTERESTS	Computational & Environmental Chemistry <ul style="list-style-type: none">• Structure, energetics, and reactivity of environmentally important compounds• Catalytic reactions on metal oxide clusters• Transition states and electron transfer	
EDUCATION	Louisiana State University (LSU) Baton Rouge, LA Ph.D., Physical/Computational Chemistry, December 2013 <ul style="list-style-type: none">• Thesis Topic: <i>Experimental & Computational Studies of Environmentally Persistent Free Radicals (EPFRs) Formation</i>• Advisors: Barry Dellinger, Ph.D and Randall Hall, Ph.D Kenyatta University (KU) Nairobi, Kenya M.Sc., Chemistry, December 2009 <ul style="list-style-type: none">• Topic: <i>Prediction of Reaction Mechanism & Absolute Rate Constant Using Computer Algorithm: The Bromate Ion in Acidic Media Reaction</i>• Advisor: Gerald Muthakia, Ph.D B.Sc., Chemistry (<i>Hons</i>), December 2004	
RESEARCH EXPERIENCE	Research Assistant	January 2010 to December 2013
	Molecular modeling and <i>ab initio</i> calculations of metal oxide clusters, reactions of metal oxide clusters with organic compounds such as phenol and chlorinated phenols, molecular orbital calculations of EPR and NMR shielding and other interactions, Time-Dependent Density Functional Theory (TDDFT), Bader charge analysis of electron distribution and electron transfer Synthesis of CuO nanoparticles supported on SiO ₂ by incipient wetness, characterization of the material using High resolution transmission electron microscopy (HRTEM and X-ray photoelectron spectroscopy (XPS). Formation of persistent free radicals on CuO/SiO ₂ , study of hydroxyl radicals (by spin trapping), study of radicals in tar balls using Electron paramagnetic resonance (EPR) spectroscopy, Extraction and Analysis by GC-MS, Radical decay studies Collaborated in development and execution of SAGA-based Pilot job over Louisiana Optical Network Initiative (LONI) and other supercomputing platforms Providing <i>ab initio</i> computational results to compliment experimental observations from experimental groups	

Supervised and mentored an undergraduate student - Taylor Hodgkins, undertaking research project in the laboratory (2013)

Supervised and trained a graduate student - Elisabeth Feld (2013)

TEACHING
EXPERIENCE

Lecturer January 2014 - to-date
Chemistry Department, Kenyatta University

Teaching undergraduate level courses: Computational Chemistry & Inorganic chemistry

Mentoring students. At Kenyatta University, I have been assigned two second year students who I am mentoring.

Teaching Assistant August 2009 - May 2010
Chemistry Department, Louisiana State University

Selected to TA general chemistry for two semesters; introducing basic concepts in Quantum Chemistry and Thermodynamics. A key responsibility was to motivate students towards scientific research.

Assistant Lecturer January 2008 to 2009
Chemistry Department, Mount Kenya University

Teaching undergraduate level courses: Physical Chemistry, Theory of spectroscopy, Unit operations I, & Organic chemistry

Mentoring students. For the few years I worked at Chemistry Department, Mount Kenya University, Kenya, my contribution in students mentorship led to the dramatic improvement of their performance

Teaching Assistant January 2007 to 2009
Department, Kenyatta University

Grading Physical Chemistry laboratory reports

SKILLS &
COMPETENCES

Certification in Best Practices in Scientific Teaching in Science, Technology, Engineering, and Mathematics (STEM).

Student/Postdoc/Alumni Network (SPAN) Leadership Committee/Training Core Leaders, 2012 - present

Softwares: GAMESS-US, Gaussian03/09, NWChem, Spartan, GRRM, WIEN2k, ORCA, Igor Pro, OriginLab

Data Visualization (VMD, Jmol, GaussView, Molden, Avogadro)

Operating Systems: Unix/Linux, Windows

Tools: Word, Excel, Powerpoint, L^AT_EX

Instruments: Electron Paramagnetic Resonance (EPR), Gas Chromatography Mass Spectrometry (GC-MS), Fourier Transform Infrared Spectroscopy (FTIR), UV-Vs Spectroscopy

AWARDS & HONORS Advancing Science Award, NOBCCChE, USA, 2013
 Graduate Enhancement award, Louisiana State University, USA, 2009
 Graduate Award, Louisiana Alliance for Simulation Guided Materials Application (LA-SiGMA) 2013
 Kenyatta University scholarship, 2006

PROFESSIONAL MEMBERSHIP Kenya Chemical Society (KCS)
 Louisiana Academy of Science (LAS), USA
 National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCCChE)

OUTREACH ENGAGEMENTS As a graduate student in Chemistry department, I volunteered at Super Science Saturday at LSU, October 19, 2013. The event is part of Chemistry department Outreach. Over 1,000 K-12 students attended the event, where campus and community groups taught students and their parents about science.
 Volunteered at the LA-SiGMA NanoDay event at the LA Arts and Science Museum, April 6, 2013. NanoDays is a nationwide festival celebrating the science of ultra-small matter.
 As a member of LA-SiGMA, I volunteered at Super Science Saturday at LSU, October 26, 2012. This event is part of LA-SiGMAs Outreach. Over 1,000 K-12 students attended the event, where campus and community groups taught students and their parents about science.

REFEREED JOURNAL PUBLICATIONS **Lucy W. Kiruri**, Barry Dellinger, B. R. Ramachandran, and Randall W. Hall. Environmentally Persistent Free Radical Formation over Aluminum Oxide Clusters: A Theoretical study. (*Manuscript Submitted in J. Phys. Chem.*)
 Gyun-Tack Bae, **Lucy W. Kiruri**, Barry Dellinger, and Randall Hall. Computational Modeling of the Initial Steps in Copper Oxide-Catalyzed Formation of Poly-Chlorinated Dibenzo Dioxins and Furans. (*Manuscript Submitted in Environmental science & technology*)
 Noureen Siraj, Farhana Hasan, Susmita Das, **Lucy W. Kiruri**, Karen E. Steege Gall, Gary A. Baker, and Isiah Warner. Carbazole-derived GUMBOS: solid state fluorescent analogs of ionic liquids for potential applications in organic-based blue light-emitting diodes. (*J. Phys. Chem. C, Article ASAP DOI: 10.1021/jp410784v*)
 James R. Reed, George F. Cawley, Taylor G. Ardoin, Barry Dellinger, Slawomir M. Lomnicki, Farhana Hasan, **Lucy W. Kiruri**, and Wayne L. Backes. Environmentally Persistent Free Radicals Inhibit Cytochromes P450 Activity in Rat Liver Microsomes. *Toxicol Appl Pharmacol. Doi: 10.1016/j.taap.2014.03.021.*

Lucy W. Kiruri, Lavrent Khachatryan, Barry Dellinger, and Slawo Lomnicki. Effect of Copper Oxide Concentration on the Formation and Persistency of Environmentally Persistent Free Radicals (EPFRs) in Particulates *Environ. Sci. Technol.* 48 (4): 22122217. Doi: 10.1021/es404013g. PMID: PMC3983329

Lucy W. Kiruri, Barry Dellinger, and Slawo Lomnicki (2013). Tar Balls from Deep Water Horizon Oil Spill: Environmentally Persistent Free Radicals (EPFR) Formation During Crude Weathering. *Environmental Science & Technology*. 47(9), 42204226

Patterson, M. C., Keilbart, N. D., **Kiruri, L. W.**, Thibodeaux, C. A., Lomnicki, S., Kurtz, R. L., Poliakoff, E. D., Dellinger, B., Sprunger, P. T. (2013). EPFR formation from phenol adsorption on Al₂O₃ and TiO₂: EPR and EELS studies *Chemical Physics* 422(0), 277282

Sarah Mahne, Gin C. Chuang, Edward Pankey, **Lucy Kiruri**, Philip J. Kadowitz, Barry Dellinger, and Kurt J. Varner (2012). Environmentally persistent free radicals decrease cardiac function and increase pulmonary artery pressure. *Am J Physiol Heart Circ Physiol.* 303, H1135H1142

PUBLISHED **Lucy W. Kiruri**, Gyun-Tack Bae, Barry Dellinger, and Randall Hall. A DFT Study of the Reaction of Chlorinated Phenols with Copper Oxide Clusters. *Proceedings of Louisiana EPSCoR RII LA-SiGMA Symposium, 1-5, 2012*

CONFERENCE **Lucy W. Kiruri**, Barry Dellinger, and Randy Hall (February 22nd, 2014). PRESENTATIONS Formation and Stabilization of Environmentally Persistent Free Radicals (EPFRs) A DFT study. *Kenya Chemical Society, AGM/WORKSHOP held at School of Physical Sciences Boardroom, Chiromo Campus, University of Nairobi.*

Lucy W. Kiruri, Slawo Lomnicki, and Barry Dellinger, (October 15 – 17, 2013). Effects of Metal Concentration on EPFRs Yield, Persistency, and OH Radical Generation. *Superfund Research Program 2013 Annual Meeting Hilton Baton Rouge Capitol Center, Baton Rouge, LA (USA).*

Lucy W. Kiruri, Barry Dellinger, and Randall Hall (June 14th, 2013). The Extent of Copper Reduction during Formation of EPFRs: A DFT study. *Invited talk at Louisiana State University, Baton Rouge, LA (USA).*

Lucy W. Kiruri, Barry Dellinger, and Randall Hall (June 12 – 13, 2013). A density functional study of the reactions of 2-Chlorophenol, 1, 2-Dichlorobenzene, Chlorobenzene with CuO - Cu₈O₈ clusters. *2nd Annual Annual High Performance Computing User Symposium, Louisiana State University - Baton Rouge, LA (USA).*

Lucy W. Kiruri, Barry Dellinger, and Slawo Lomnicki (May, 14 – 18, 2013). Effect of Cu(II)O concentration in Cu(II)O/Silica particles on the formation of environmentally persistent free radicals (EPFRs) and reactive oxygen species (ROS). *13th International Congress on Combustion By-Products and their Health Effects, New Orleans, LA (USA).*

Slawo Lomnicki, **Lucy W. Kiruri**, and Barry Dellinger (May, 14 – 18, 2013).

Persistent Radicals in Tar Balls. Paper presented by Slawo M. Lomnicki at the *13th International Congress on Combustion By-Products and their Health Effects, New Orleans, LA (USA)*.

Slawo M. Lomnicki, **Lucy Kiruri**, Barry H. Dellinger (November 4 – 6, 2012). Lifetime and Stability of Environmentally Persistent Free Radicals-What matters? Paper presented by Slawo M. Lomnicki at the *Southwest Regional ACS Meeting Baton Rouge, LA (USA)*.

Kurt J Varner, Sarah Mahne, Gin Chuang, Edward Pankey, **Lucy Kiruri**, Barry Dellinger (November 4 – 6, 2012). Environmentally Persistent Free Radicals Decrease Cardiac Function In Vivo. Paper presented by Kurt J. Varner at the *Southwest Regional ACS Meeting Baton Rouge, LA (USA)*.

Lucy W. Kiruri, Barry Dellinger, and Slawo Lomnicki (October 21 – 24, 2012). Formation And Stabilization Of Combustion-Generated, Environmentally Persistent Radicals On Alumina Surfaces. *The 25th Annual Meeting of the Superfund Research Program Marriot City Center - Raleigh, NC (USA)*.

Lucy W. Kiruri, Gyun-Tack Bae, Barry Dellinger, and Randall Hall (July, 2012). Copper Oxide-Cluster Model of Environmentally Persistent Free Radicals Formation. *LA-SiGMA & LA-EPSCoR Annual Symposium, Baton Rouge, LA (USA)*.

Lucy W. Kiruri, Barry Dellinger, and Randall Hall (July, 2012). Global Reaction Route Mapping (GRRM): Study of Al₂O₃ Isomers. Paper presented at the 2nd Annual LA-SiGMA Graduate Students Retreat, Tulane University, LA (USA).

Cheri A. McFerrin, **Lucy W. Kiruri**, Gyun-Tack Bae, Collin D. Wick, and Randall W. Hall (October, 2011). Modeling of Role of Copper Oxide Clusters in Pollutant Formation. Paper presented by Cheri A. McFerrin at the *20th Conference on Current Trends in Computational Chemistry, Jackson, Mississippi (USA)*.

Lucy W. Kiruri, Barry Dellinger, and Slawo Lomnicki (June, 2011). Environmentally Persistent Free Radicals in Soot and Bottom Ash from Controlled Wood Burning. *12th International Congress on Combustion By-Products and their Health Effects, Hangzhou, China*.

Lucy W. Kiruri, Gyun-Tack Bae, Barry Dellinger, and Randall Hall (June, 2011). *Ab initio* Studies of Reactions of Phenol and Chlorinated Phenols with Copper Oxide Clusters. *12th International Congress on Combustion By-Products and their Health Effects, Hangzhou, China*.

Slawo Lomnicki, Eric Vejerano, **Lucy Kiruri**, Barry Dellinger, and (June, 2011). Transition Metal Ions and Environmentally Persistent Free Radicals. Paper presented by Slawo M. Lomnicki at the *12th International Congress on Combustion By-Products and their Health Effects, Hangzhou, China*.

2nd Annual High Performance Computing User Symposium, June 12–13th, 2013, Louisiana State University, Baton Rouge, LA (USA).

Understanding and meeting information and technology needs to prevent exposures to engineered nanoparticles, June 5–7th, 2013, Southeastern Louisiana University, Hammond, LA (USA).

LA-SiGMA All-hands Meetings, EPSCoR RII, July 23rd, 2012, Baton Rouge, LA (USA).

NWChem Workshop, June 8-9th, 2012, Louisiana State University, Baton Rouge, LA (USA). Presenters: Eric Bylaska and Hub van Dam, main code developers.

LA-SiGMA All-hands Meetings, EPSCoR RII, August 5th, 2011, Louisiana Board of Reagents, Baton Rouge, LA (USA).

LA-SiGMA All-hands Meetings, EPSCoR RII, June 20th, 2011, Louisiana Board of Reagents, Baton Rouge, LA (USA).

Introduction to Computational Thinking Workshop, July 31st- August 6th, 2011, Louisiana State University, Baton Rouge, LA (USA).

Density Functional Theory Workshop, July 23rd-27th, 2011, Louisiana State University, Baton Rouge, LA, (USA).

The Kenya Chemical Society (Nairobi Chapter), August 30th, 2008, University of Nairobi, Kenya.

DOCTORATE
COURSEWORK

- Computational Chemistry
- Introduction to Maths Chemistry & 3D visualization
- Introduction to Quantum Chemistry
- Introduction to Statistical Thermodynamics
- Mass Spectrometry
- Molecular Spectroscopy

REFEREES

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