Emilie Guidez, Ph.D.

University of Colorado Denver
Phone: 303-315-7691
E-Mail: emilie.guidez@ucdenver.edu

Education

- **Ph.D. in Chemistry**, Kansas State University, Manhattan, KS 2009-2014
  Major Professor: Pr. Christine M. Aikens
  Dissertation title: *Quantum Mechanical Origin of the Plasmonic Properties of Noble Metal Nanoparticles.*
- **B.S. in Chemistry**, University of Geneva, Geneva Switzerland. 2005-2008

Professional positions

- **Assistant Professor of Chemistry**, University of Colorado Denver, Denver, CO Since August 2017
- **Postdoctoral Research Associate**, Iowa State University, Ames, IA 2014-2017
  Major Professor: Pr. Mark S. Gordon.
- **Graduate Research Assistant**, Kansas State University, Manhattan, KS 2010-2014
- **Graduate Teaching Assistant**, Kansas State University, Manhattan, KS Fall 2009-Fall 2010

Research activities

Identify how the chemical environment (solvent and ligand shell) of metallic nanoparticles affects their optical and chemical properties so that these properties can be tuned for applications in cancer therapy, clean energy generation, catalysis and other nanotechnologies. Standard quantum mechanical methods are used and new methods developed to model these systems.

Past Research Activities

❖ Postdoctoral Research

- Investigating the non-linear structure of Si_2H_2 isomers using localized molecular orbital theory and a new energy decomposition analysis scheme by Pr. Klaus Ruedenberg. This project is in collaboration with Pr. Klaus Ruedenberg and Dr. Aaron West at Iowa State University.
- Development of a new method combining quantum mechanics and molecular mechanics to compute the free energies of host-guest complexes. This project involves the combination of the GAMESS and VM2 software. This project is in

collaboration with Dr. Peng Xu and Dr. Tosaporn Sattasathuchana at Iowa State University, Dr. Dr. Simon Webb at VeraChem, LLC.

- Development of a new effective fragment potential for water including dispersion interactions (EFP1-D).
- Investigating the importance of the E^7 dispersion energy term on liquids of increasing viscosities.
- Evaluating solvent effects on the catalytic properties of mesoporous silica nanoparticles using fragmentation methods. This project is in collaboration with Professor Igor Slowing at Iowa State University.
- Evaluating Enzyme I mechanism using fragmentation methods. This project is in collaboration with Professor Vincenzo Venditti at Iowa State University.
- Deriving and implementing a many-body dispersion energy term in the Effective Fragment Potential method.
- Implemented a non-parameterized dispersion correction into the Density Functional Theory code in the GAMESS package.
- Derived the gradient of the odd dispersion energy term E^7 and implemented it in GAMESS.

❖ *Graduate Research*

- Simulated the Magnetic Circular Dichroism spectrum of the thiolate-protected gold nanoparticle $Au_{25}(SR)_{18}^-$ using Time-Dependent Density Functional Theory.
- Examined the origin of the emission of the $Au_{38}(SR)_{24}$ cluster using *ab initio* molecular dynamics simulations.
- Performed molecular dynamics simulations to investigate the potential isomerization of the $Au_{38}(SR)_{24}$ complex.
- Evaluated doping energies of cadmium selenide clusters with gallium, indium and tin to investigate their stability and their effect on quantum dot formation. This work is in collaboration with the experimental group of Pr. Viktor Chikan at Kansas State University.
- Investigated the origin of the luminescence of the gold-thiolate complex $(TPA)AuSCH(CH_3)_2$.
- Examined the origin of plasmon resonances in linear polycyclic aromatic hydrocarbons and compared them to plasmon resonances in noble metal nanoparticles. Benchmarked a variety of exchange-correlation functionals to calculate plasmons in polycyclic aromatic hydrocarbons.
- Developed a configuration interaction model to describe plasmon resonances.
- Determined the effect of silver doping on the absorption spectrum of the gold nanoparticle $Au_{25}(SR)_{18}^-$ in collaboration with Prof. Hannu Häkkinen's group (University of Jyväskylä, Finland).

- Developed a program in Fortran to calculate energy levels of ligand-protected spherical gold nanoparticles based on a charge-perturbed particle in a sphere model.
- Calculated absorption spectra of gold and silver nanowires and nanorods using Time-Dependent Density Functional Theory. Evaluated length and diameter effects on the absorption spectrum.
- Investigated the growth mechanism of gold-phosphine nanoparticles with Density Functional Theory.

Teaching Experience

❖ Graduate Courses

- Guest lecturer for the quantum chemistry class at Iowa State University (3 sessions Spring 2016 and 4 sessions Spring 2017). — Spring 2016, Spring 2017
- Guest lecturer for the group theory class at Iowa State University (3 sessions in Spring 2017 and 4 sessions in Spring 2016). — Spring 2016, Spring 2017
- Guest lecturer for computational chemistry at Iowa State University (half a semester). — Fall 2015
- Guest lecturer for the graduate computational chemistry course at Kansas State University (1 session). — Summer 2013

❖ Undergraduate Courses

- Guest lecturer for general chemistry at Iowa State University (1 session). — Fall 2015
- Guest lecturer for physical chemistry I (thermodynamics, kinetics) undergraduate course at Kansas State University. (2 sessions) — Fall 2013
- Guest lecturer for the physical chemistry II (quantum mechanics, spectroscopy) undergraduate course at Kansas State University (2 sessions). — Spring 2013
- Graduate teaching assistant for Freshman Chemistry laboratory at Kansas State University. — Fall 2009/Fall 2010

❖ Other instructional activities

- Teaching-as-research project (funding $625): Redesigning chemistry homework assignments to improve material retention — Fall 2016

- Basic language training instructor (French) at Kansas State University: Designed curriculum, taught class to ten students. — Spring 2013

Awards and Achievements

- Center for the Integration of Research Teaching and Learning (CIRTL) associate. — Spring 2017
- Massive open online course from the Center for the Integration of Research Teaching and Learning (CIRTL): Advancing learning through evidence based STEM teaching. — Summer 2016
- Wiley computers in chemistry outstanding postdoc award, American Chemical Society, COMP division — Fall 2016
- Kansas State University Chemistry Department Research award. — April 2014
- International Coordinating Council scholarship. — April 2013
- Chemical Computing Group Excellence award, American Chemical Society COMP division. — August 2012
- Journal of Physical Chemistry award for Graduate Research, Telluride CO. — July 2012
- Peter Salomon award to attend the Telluride School on Theoretical Chemistry, Telluride CO. — July 2012
- Phi Lambda Upsilon Graduate Research excellence award. — April 2012

Publications

1. Photoluminescence Origin of $Au_{38}(SR)_{24}$ and $Au_{22}(SR)_{18}$ Nanoparticles: A Theoretical Perspective. Dimuthu K. L. Weerawardene, Emilie B Guidez and Christine M. Aikens, *The Journal of Physical Chemistry C*, submitted.
2. Dispersion interactions in water clusters. Emilie B Guidez and Mark S. Gordon, *The Journal of Physical Chemistry A*, just accepted.
3. Derivation and implementation of the gradient of the R^{-7} dispersion interaction in the effective fragment potential method. Emilie B. Guidez, Peng Xu and Mark S. Gordon, *The Journal of Physical Chemistry A*, DOI: 10.1021/acs.jpca.5b11042.
4. Synthesis and Characterization of Gallium-Doped CdSe Quantum Dots. Hongfu Luo, Christopher Tuinenga, Emilie B. Guidez, Christopher Lewis, Josh Shipman, Santanu Roy, Christine M. Aikens and Viktor Chikan, *The Journal of Physical Chemistry C*, **2015**, *119 (19)*,10749-10757
5. Time-Dependent Density Functional Theory Study of the Luminescence Properties of Gold Phosphine Thiolate Complexes. Emilie B. Guidez and

Christine M. Aikens, *The Journal of Physical Chemistry A*, **2015**, *119 (14)*, 3337-3347

6. A Dispersion Correction Derived from First-Principles for Density Functional Theory and Hartree Fock Theory. Emilie B. Guidez and Mark S. Gordon, *The Journal of Physical Chemistry A*, **2015**, *119 (10)*, 2161-2168
7. Quantum Mechanical Origin of the Plasmon: From Molecular Systems to Nanoparticles. Emilie B. Guidez and Christine M. Aikens, *Nanoscale,* **2014**, *6* (20), 11512-11527 (feature article)
8. Quantum coherent plasmon in silver nanowires: A real-time TDDFT study. Feizhi Ding, Emilie B. Guidez, Christine M. Aikens and Xiaosong Li, *The Journal of Chemical Physics*, **2014**, *140*, 244705
9. Plasmon Resonance Analysis with Configuration Interaction. Emilie B. Guidez and Christine M. Aikens, *Physical Chemistry Chemical Physics,* **2014**, *16*, 15501-15509
10. Origin and TDDFT Benchmarking of the Plasmon Resonance in Acenes. Emilie B. Guidez and Christine M. Aikens, *The Journal of Physical Chemistry C*, **2013**, *117* (41), 21466-21475
11. Diameter-Dependence of the Excitation Spectra of Silver and Gold Nanorods. Emilie B. Guidez and Christine M. Aikens, *The Journal of Physical Chemistry C*, **2013**, *117* (23), 12325–12336
12. Effects of Silver Doping on the Geometric and Electronic Structure and Optical Absorption Spectra of the $Au_{25-n}Ag_n(SH)_{18}^-$ (n = 1, 2, 4, 6, 8, 10, 12) Bimetallic Nanoclusters. Emilie B. Guidez, Ville Mäkinen, Hannu Häkkinen, and Christine M. Aikens, *The Journal of Physical Chemistry C*, **2012**, *116* (38), 20617–20624
13. Theoretical Analysis of the Optical Excitation Spectra of Silver and Gold Nanowires. Emilie B. Guidez and Christine M. Aikens, *Nanoscale*, **2012**, *4*, 4190-4198
14. Development of a Charge-Perturbed Particle-in-a-Sphere Model for Nanoparticle Electronic Structure. Emilie B. Guidez and Christine M. Aikens, *Physical Chemistry Chemical Physics*, **2012**, *14* (12), 4287–4295
15. Initial Growth Mechanisms of Gold-Phosphine Clusters. Emilie B. Guidez, Allison Hadley, and Christine M. Aikens, *The Journal of Physical Chemistry C*, **2011**, *115* (14), 6305-6316

Professional Presentations

❖ *Oral Presentations*

- Bonding analysis of the Si_2H_2 isomers. Emilie B Guidez, Mark S. Gordon and Klaus Ruedenberg. **GAMESS7557 Symposium**, Kauai, Hawaii, January 16th-18th,2017

- Time-Dependent Density Functional Theory (TDDFT) Study of the Luminescence Properties of Phosphine Gold (I) Thiolate Complexes. Emilie B. Guidez and Christine M. Aikens, **ACS National Meeting**, Denver, CO, March 22nd-26th, 2015
- Configuration Interaction Approach to Plasmon Resonances in Acenes and Noble Metal Nanoparticles. Emilie B. Guidez and Christine M. Aikens, **IGERT Symposium**, Sioux Falls, SD, Oct 4th, 2014 (invited lecture)
- Configuration Interaction Approach to Plasmon Resonances in Acenes and Noble Metal Nanoparticles. Emilie B. Guidez and Christine M. Aikens, **ACS National Meeting**, Dallas, TX, March 16th-21st, 2014
- Configuration Interaction Approach to Plasmon Resonances. Emilie B. Guidez and Christine M. Aikens, **Kansas Physical Chemistry Symposium**, Lawrence, KS, November 9th, 2013
- Effects of Silver Doping on the Geometric, Electronic Structure and Optical Absorption Spectra of the $Au_{25-n}Ag_n(SH)_{18}^-$ (n = 1, 2, 4, 6, 8, 10, 12) Bimetallic Nanoclusters. Emilie B. Guidez and Christine M. Aikens, **ACS Midwest Regional Meeting**, Omaha, NE, October 24th-26th, 2012
- Effects of Silver Doping on the Geometric, Electronic Structure and Optical Absorption Spectra of the $Au_{25-n}Ag_n(SH)_{18}^-$ (n = 1, 2, 4, 6, 8, 10, 12) Bimetallic Nanoclusters. Emilie B. Guidez and Christine M. Aikens, **Kansas Physical Chemistry Symposium**, Manhattan, KS, October 13th, 2012
- Calculating the Electronic Structure of Spherical Ligand-Protected Gold Nanoparticles using a Charge-Perturbed Particle-in-a-Sphere Model. Emilie B. Guidez and Christine M. Aikens, **American Chemical Society National Meeting**, Exploring Potential Energy Surfaces in Quantum Chemistry: A Tribute to H. Bernhard Schlegel, Philadelphia, PA, August 19th-23rd , 2012
- Development of a Charge-Perturbed Particle-in-a-sphere Model for Electronic Structure Calculations of Ligand-Protected Gold Nanoparticles. Emilie B. Guidez and Christine M. Aikens, **Nanomaterials: Theory and Computation Workshop**, Telluride, CO, July 16th-20th, 2012
- Initial Growth Mechanisms of Gold-Phosphine Clusters. Emilie B. Guidez and Christine M. Aikens, **Kansas Physical Chemistry Symposium**, Kansas State University, Manhattan, KS, November 13th, 2010

❖ *Poster Presentations*

- Odd order dispersion interactions in water clusters. Emilie B. Guidez and Mark S. Gordon, **GAMESS7557 Symposium**, Kauai, Hawaii, January 16th-18th,2017
- Odd order dispersion interactions in water clusters. Emilie B. Guidez and Mark S. Gordon, **Theory and Applications of Computational Chemistry**, Seattle, WA, August 28th- September 2nd, 2016
- Odd order dispersion interactions in water clusters. Emilie B. Guidez and Mark S. Gordon, **American Chemical Society National Meeting**, Philadelphia, PA, August 21st-25th, 2016

- Effective fragment potential dispersion correction to Density Functional Theory and Hartree-Fock Theory. Emilie B. Guidez and Mark S. Gordon, **Intermolecular interactions workshop**, Telluride, CO, July 6th-12th, 2015
- Origin and TDDFT Benchmarking of the Plasmon Resonance in linear polycyclic aromatic hydrocarbons. Emilie B. Guidez and Christine M. Aikens, **Midwest Theoretical Chemistry Conference**, Urbana, IL, May 29th-31st, 2013
- Development of a Charge-Perturbed Particle-in-a-sphere Model for Electronic Structure Calculations of Ligand-protected Gold Nanoparticles. Emilie B. Guidez and Christine M. Aikens, **American Chemical Society National Meeting**, Chemical Computing Group Excellence Award, Philadelphia, PA, August 19th-23rd , 2012
- Development of a Charge-Perturbed Particle-in-a-Sphere Model for Electronic Structure Calculations of Ligand-protected Gold Nanoparticles. Emilie B. Guidez and Christine M. Aikens, **International Congress on Quantum Chemistry**, University of Colorado, Boulder, CO, June 25th-30th, 2012
- Theoretical Analysis of the Optical Excitation Spectra of Silver and Gold Nanowires. Emilie B. Guidez and Christine M. Aikens, **Kansas Physical Chemistry Symposium**, University of Kansas, Lawrence, KS, November 19th, 2011
- Theoretical Analysis of the Optical Excitation Spectra of Silver and Gold Nanowires. Emilie B. Guidez and Christine M. Aikens, **American Chemical Society Midwest/Great Lakes Regional Meeting**, St-Louis, MO, October 19th-22nd, 2011
- Development of a Charge-Perturbed Particle-in-a-Sphere Model for Nanoparticle Electronic Structure. Emilie B. Guidez and Christine M. Aikens, **American Conference on Theoretical Chemistry**, Telluride, CO, July 17th-22nd, 2011

Service

❖ *Professional and Institutional*

- **Reviewer for the journal *Physica B*** — Since March 2017
- **Reviewer for *The Journal of Physical Chemistry*** — Since November 2016
- **Reviewer for the journals *Physical Chemistry Chemical Physics* and *Nanoscale*** — Since March 2016
- **President of the Iowa State University Postdoctoral Association.** — 2015-2016
  Responsibilities and achievements: communicating with the Dean of the graduate college about issues faced by postdocs, organizing and overseeing the social activities and professional development seminars organized by the association, running committee meetings. Updated the constitution.

- **Postdoc representative in Iowa State University Committee on Women.** March 2015-August 2017
  Responsibilities: Addressing gender inequality issues in the postdoctoral community. Member of the Liberal Arts and Science review committee, whose purpose is to provide a comprehensive and objective analysis of data on the status of women at the college level for the purpose of developing strategies to ensure equality and diversity.
- **Secretary of the Iowa State University Postdoctoral Association.** 2014-2015
  Responsibilities: Organizing meetings, taking meeting minutes, preparing meeting agenda, preparing general meeting announcements, co-organizing the Midwest postdoctoral symposium.
- **Graduate and Professional Student Research Conference committee member** at Iowa State. October 2014-April 2015
  Responsibilities: recruiting postdoc judges for poster and oral presentations and for evaluating abstracts, setting evaluation criteria for the submitted abstracts and presented talks.

Affiliations and Memberships

- American Association for the Advancement of Science (AAAS) Since 2016
- American Chemical Society computational division Since 2012
- American Chemical Society (ACS) Since 2011
- Phi Kappa Phi Society, Kansas State University chapter Since 2011
- Phi Lambda Upsilon, Alpha Epsilon chapter Since 2010

Programs and Software

- ADF, GAMESS, VASP, NWChem, QChem, Matlab, Fortran, Python, Microsoft Office (Word, PowerPoint, Excel)