

## Olaseni Sode

### Work Address:

5735 S. Ellis Ave.  
Searle 231  
The University of Chicago  
Chicago, IL 60615

oosode@uchicago.edu  
+1 (314) 856-2373

### Home Address:

1119 E Hyde Park Blvd  
Apt. 3E  
Chicago, IL 60615

olaseni.sode@gmail.com  
+1 (314) 856-2373  
<http://www.olaseniosode.com>

## Education

University of Illinois at Urbana-Champaign  
Ph.D. in Chemistry  
Urbana, IL  
September 2012

- Supervisor: Professor So Hirata
- Thesis title: A Theoretical Study of Molecular Crystals
- Transferred from the University of Florida in 2010 with Prof. Hirata

Morehouse College  
B.S. & B.A. in Chemistry and French  
Atlanta, GA  
December 2006

- Studied at the Université de Nantes, Nantes, France (2004-2005)

## Research Experience

The University of Chicago  
Postdoctoral Research – research advisor: Dr. Gregory A. Voth  
Chicago, IL  
2012–present

- Studied proposed proton transport minimum free-energy pathways in [FeFe]-hydrogenase via molecular dynamics simulations and the multistate empirical valence bond technique.
- Collaborated to develop the multiscale string method to accelerate refinement of chemical reaction pathways of adenosine triphosphate (ATP) hydrolysis in globular and filamentous actin proteins.

University of California, San Diego  
Visiting Scholar – research advisor: Dr. Francesco Paesani  
La Jolla, CA  
2014, 2015

- Developed and implemented a reactive molecular dynamics scheme for condensed phase systems of the hydrated hydronium ions.

University of Illinois at Urbana-Champaign  
Doctoral Research – research advisor: Dr. So Hirata  
Urbana, IL  
2010-2012

- Characterized the vibrational structure of extended systems including infrared and Raman-active vibrations, as well as phonon dispersions and densities of states in the first Brillouin zone.
- Developed zero-point vibrational energy analysis scheme for molecular clusters using a fragmented, local basis scheme.

University of Florida  
Doctoral Research – research advisor: Dr. So Hirata  
Gainesville, FL  
2007–2010

- Studied the structural parameters of molecular crystals such as hydrogen fluoride, carbon dioxide, and phases of ice, including finite pressure effects using ab initio quantum chemistry calculations.

Morehouse College  
Atlanta, GA

Undergraduate Research – research advisor: Dr. John Hall 2006–2007

- Performed computational investigation of alpha-D-glucosamine with Spartan quantum chemistry software package.

Université de Toulouse Toulouse, France  
Undergraduate Research – research advisor: Dr. Alain Igau 2005

- Synthesized adaptive ligand precursor proposed by the Igau research team for solar cell application.

Georgia Institute of Technology Atlanta, GA  
Undergraduate Research – research advisor: Dr. Laren Tolbert 2004

- Investigated the photo-induced proton transfer in 1-Methyl-6-Hydroxyquinolinium Triflate with UV/Vis and fluorescence spectroscopy.

## Publications

- J. Li, **O. Sode** and S. Hirata, ‘Second-order many-body perturbation study of thermal expansion of solid carbon dioxide,’ *J. Chem. Theory Comput.* 11, 224 (2015).
- S. Kale, **O. Sode**, J. Weare and A. Dinner, ‘Finding Chemical Reaction Paths with a Multilevel Preconditioning Protocol,’ *J. Chem. Theory Comput.* 10, 5467 (2014).
- **O. Sode** and G.A. Voth, ‘Electron Transfer Activation of a Second Water Channel for Proton Transport in [FeFe]-Hydrogenase,’ *J. Chem. Phys.* 141, 22D527 (2014).
- S. Hirata, **O. Sode**, M. Keçeli, K. Yagi and J. Li, ‘Response to Comment on Fermi resonance in solid CO<sub>2</sub> under pressure,’ *J. Chem. Phys.* 140, 177102 (2014).
- K. Gilliard, **O. Sode** and S. Hirata, ‘Second-order many-body perturbation and coupled-cluster singles and doubles study of ice VIII,’ *J. Chem. Phys.* 140, 174507 (2014).
- S. Hirata, K. Gilliard, X. He, J. Li and **O. Sode**, ‘Ab Initio Molecular Crystal Structures, Spectra, and Phase Diagrams,’ *Accounts Chem. Res.* 47, 2721 (2014).
- J. Li, **O. Sode**, G. A. Voth, and S. Hirata, ‘Ab Initio Study of A Solid-Solid Phase Transition in Carbon Dioxide at High Pressures and Intermediate Temperatures,’ *Nature Comm.* 4, 2647 (2013).
- **O. Sode**, M. Keçeli, K. Yagi, and S. Hirata, ‘Fermi resonance in solid CO<sub>2</sub> under pressure,’ *J. Chem. Phys.* 138, 074501 (2013).
- X. He, **O. Sode**, S. Xantheas and S. Hirata, ‘Second-order many-body perturbation study of ice Ih,’ *J. Chem. Phys.* 137, 204505 (2012).
- **O. Sode** and S. Hirata, ‘Embedded fragmentation of vibrational frequencies,’ *J. Chem. Phys.* 137, 174104 (2012).
- **O. Sode** and S. Hirata, ‘Second-Order Many-body Perturbation Study of Solid Hydrogen Fluoride Under Pressure,’ *Phys. Chem. Chem. Phys.* 14, 7765 (2012).
- **O. Sode** and S. Hirata, ‘Second-Order Many-Body Perturbation Study of Solid Hydrogen Fluoride,’ *J. Phys. Chem. A.* 114, 8873 (2010).
- **O. Sode**, M. Keçeli, S. Hirata, and K. Yagi, ‘Coupled-Cluster and Many-Body Perturbation Study of Energies, Structures, and Phonon Dispersions of Solid Hydrogen Fluoride,’ *Int. J. Quantum Chem.* 109, 1928 (2009).

## Book Chapters

- S. Hirata, M. Keçeli, Y.-Y. Ohnishi, **O. Sode** and K. Yagi, ‘Extensivity of Energy and Size-Consistent Electronic and Vibrational Structure Methods for Crystals,’ *Annu. Rev. Phys. Chem.* 63, 131-153 (2012).

## Olaseni Sode

- S. Hirata, **O. Sode**, M. Keçeli and T. Shimazaki, 'Electron Correlation in Solids: Delocalized and Localized Orbital Approaches,' a chapter in *Accurate Condensed-Phase Quantum Chemistry* edited by F. Manby, p.129-161 (CRC Press, Boca Raton, 2010).

### Conferences and Workshops

- Postdoc to PUI Professor Workshop, Hope College, Holland, MI, April 2015.
- Oral presentation, Association of American Colleges and Universities Annual Meeting, Washington, D.C., January 2015.
- Poster presentation, Conference of Ford Fellows, Irvine, CA, September 2014.
- Poster presentation, Midwest Theoretical Chemistry Conference, Evanston, IL, June 2014.
- Oral and poster presentation, Center for Multiscale Theory and Simulation CCI Review, National Science Foundation, Arlington, VA, March 2014.
- Oral presentation, Workshop on Multiscale Theory and Simulation, The University of Chicago, Chicago, IL, June 2013.
- Oral presentation, Chemistry Lecture Series, Morehouse College, Atlanta, GA, November 2012.
- Oral presentation, Electronic Structure Interest Group, Urbana, IL, March 2012.
- Poster presentation, Quantum Molecular Dynamics Conference, Berkeley, CA, January 2012.
- Oral presentation, ACS National Meeting, Anaheim, CA, March 2011.
- Poster presentations, Molecular Quantum Mechanics Conference, Berkeley, CA May 2010.
- Poster presentations, Sanibel Symposium in St. Simons, GA, February 2009 and 2010.
- Poster presentation, Conference on Current Trends in Computational Chemistry in Jackson, MS in 2009.

### Community Outreach

- Target H.O.P.E. Panel Discussion, Chicago, IL, May, 2014
- Project Innovation Symposium, Glen Ellyn, IL, February 2014
- Expanding Your Horizons, Chicago, IL, March 2014 and March 2013
- Science Pub Event Series, Chicago, IL, October 2013
- Career Day Demonstrations at Museum of Science and Industry, Chicago, IL, October 2013
- Seminars for Endorsement of Science and Mathematics Educators, Chicago, IL, August 2013
- Malcolm X College Annual STEM Symposium, Chicago, IL, October, 2012
- Atlanta University Center Chess Mentor Program at Lyke House Catholic Center, Atlanta, GA, 2005-2006

### Awards

- Ford Foundation Postdoctoral Fellowship in 2014 (\$40,000).
- Georgia Tech School of Chemistry & Biochemistry Focus Fellows Postdoctoral Selectee in 2014.
- CATMS travel award at the University of Illinois at Urbana-Champaign in 2011.
- University fellowship (Roger Adams Fellow) by the University of Illinois at Urbana-Champaign in 2010.

## Olaseni Sode

- GAANN fellowship at the University of Illinois at Urbana-Champaign.
- Best graduate student poster prize at the 49<sup>th</sup> Sanibel Symposium in St. Simons, GA in 2009.
- University fellowship (Alumni Fellow) by the University of Florida 2007 – 2010.
- Beta Kappa Chi (Science Honor Society) at Morehouse College in 2006.
- Member of National Society of Collegiate Scholars at Morehouse College in 2003.

### Skills and Expertise

- Postdoctoral mentor to undergraduate and high school researchers, in charge of developing research topics, introducing the molecular dynamics theory, arranging weekly meetings, and instructing the science projects.
- Author of a Python program that fragments large and extended molecular systems in order to efficiently and accurately determine their electronic and vibrational structure with methods such as HF, MP2, CC, and DFT.
  - O. Sode, BIM, University of Illinois at Urbana-Champaign, (2012).
- Experienced user of Matlab, Maple, Mathematica and quantum chemistry packages such as NWChem, Gaussian, Q-Chem, along with the molecular dynamics software NAMD, CP2K, and LAMMPS .
- Expert on Python, C++, shell scripting, all main OSs (Unix/Linux, Mac OS X, Windows) and experienced on Fortran, Java, OpenMP and MPI.
- Teaching assistant for freshman level chemistry courses (2007, 2008).
- French – proficient.

### References

- Professor Gregory A. Voth, The University of Chicago, gavoth@uchicago.edu, (773) 702-9092.
- Professor So Hirata, University of Illinois at Urbana-Champaign, sohirata@illinois.edu, (217) 244-0629.
- Professor Aaron Dinner, The University of Chicago, dinner@uchicago.edu, (773) 702-2330.