# Bing Gu

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## Education

**Ph.D. Candidate** — Current, from Aug 2011
*Department of Chemistry and Biochemistry, University of South Carolina, Columbia*

**Bachelor of Science** — Jul 2011 – Oct 2007
*Department of Physical Chemistry, University of Science and Technology of China, China*

## Research Experience

**Research Assistant** — Current, from Aug 2011
Dr. Sophya V. Garashchuk's Group
*Department of Chemistry and Biochemistry, University of South Carolina – Columbia*

**Research Assistant** — Aug 2010 – Jul 2011
Dr. Qunxiang Li's Group
*Department of Physical Chemistry, University of Science and Technology of China*

Thesis: *The Spin-PolarizationTransport properties of the M@$Au_6$ (M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni) clusters using ab-initio methods.*

## Teaching Experience

**Teaching Assistant** — Spring 2015
Thermodynamics - Chem 541
*Department of Chemistry and Biochemistry, University of South Carolina – Columbia*

**Teaching Assistant** — Spring 2014
Quantum Mechanics and Spectroscopy - Chem 542
*Department of Chemistry and Biochemistry, University of South Carolina – Columbia*

**Teaching Assistant** — Fall 2011 and Spring 2012
Physical Chemistry lab sections
*Department of Chemistry and Biochemistry, University of South Carolina, Columbia*

## Awards

- Dr. James R. Durig Graduate Student Travel Award — 2015
  *Department of Physical Chemistry, University of South Carolina, Columbia*
- Outstanding Student Scholarship — 2011
  *Department of Physical Chemistry, University of Science and Technology of China, Anhui, China*

## *Research Interests*

- Development of quantum dynamics methods scalable to large molecular systems.
- Theory and simulation of chemical reactions
- Code development and high-performance computing.

## *Additional coursework and training*

- Department of physics, University of South Carolina
  - Quantum field theory — Fall 2015
  - Quantum statistical thermodynamics — Spring 2015
- Department of mathematics, University of South Carolina
  - Foundations of Computational Algorithm I & II — Fall 2013 & Spring 2014
  - Mathematical Fluid Dynamics — Fall 2014
- NMR tutorial - Organic structure determination , *Columbia, SC* — Jan 09-15, 2015
- (SICM)2 Parallel Computing Workshop, *Stony Brook, NY* — Jul 07-19, 2014
- RCI Python Workshop, *Columbia, SC* — Feb 24-25, 2014
- OpenACC GPU Programming Remote Workshop, *Columbia, SC*, — Aug 13-14, 2013
- XSEDE MPI Workshop , *Columbia, SC* — Dec 04-05, 2013
- Openacc GPU Programming Remote Workshop, *Columbia, SC* — Aug 13-14, 2013
- Vanderbilt/Columbia Molecular Modeling Cybercamp , *Nashville, TN* — May 28–31, 2012
- Programming Heterogeneous Parallel Computing Systems, *Columbia, SC* — Jul 09-13, 2012

## *Computer and programming skills*

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| **Operating Systems** | Linux, Mac OS X, Windows |
| **Programming Languages** | Python, C/C++ Language, Fortran, MPI, OpenMP |
| **Computational Packages and Software** | Qchem, Spartan, Maple |

## Synergistic Activities

- Judge for the USC Science Fair of Midlands Region, Columbia, SC 03/2014
- Member of the American Physics Society Since 09/2014
- Member of the American Chemistry Society Since 09/2014

## Presentations

- ACS National Meeting, Denver, CO 03/16/2015
  *Quantum molecular dynamics with friction : Estimating quantum effects of atomic solids*
- Physical Chemistry Divisional Seminar
  - *Quantum molecular dynamics with friction* 02/16/2015
  - *The Zero-Point Energy Leak in Molecular Dynamics* 04/02/2012
- $81^{st}$ Annual Meeting of the APS Southeastern Section 11/15/2014
  *Estimation of quantum effects of atomic solids using quantum trajectory dynamics with dissipation*
- Physical Chemistry Divisional Seminar
- Southeast Theoretical Chemistry Association Annual Meeting
  - *Estimation of quantum effects in atomic solids using quantum trajectory dynamics with dissipation* 05/09/2014
  - *Calculation of reaction rate constant in a double-well potential* 05/10/2013

## Publications

- Bing Gu and Sophya Garashchuk, *Quantum Dynamics with Gaussian Bases Defined by the Quantum Trajectories*, J. Phys. Chem. A, DOI: 10.1021/acs.jpca.5b10029
- Bing Gu, Sophya Garashchuk, *Molecular dynamics of large systems with quantum corrections for the nuclei*, AIP Conf. Proc. **1702**, 090014 (2015)
- Bing Gu and Sophya Garashchuk, *Determination of the collective modes from the quantum-mechanical time-correlation functions*, Theo. Chem. Accounts 2015, 134:129
- Bing Gu, Robert J. Hinde, Vitaly Rassolov, Sophya Garashchuk, *Estimation of quantum mechanical effects of atomic solids with quantum trajectory method with dissipation*, J. Chem. Theory Comput., **2015**, 11 (7), pp 2891-2899
- Sophya Garashchuk, Bing Gu and James Mazzuca, *Calculation of the Quantum-Mechanical Tunneling in Bound Potentials*, J. Theo. Chem., **2014**, 240491 (2014)
- Sophya Garashchuk, Vaibhav Dixit, Bing Gu and James Mazzuca, *The Schrödinger equation with friction from the quantum trajectory perspective*, J. Chem. Phys. **138**, 054107 (2013)