Bing Gu

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Research Experience

2023 - **Assistant Professor,** Department of Chemistry, School of Science, Westlake University, Zhejiang, China

2018-2022 **Postdoctoral Fellow**, Advisor: Dr. Shaul Mukamel
Department of Chemistry & Department of Physics and Astronomy, University of California, Irvine, CA

2016-2018 **Postdoctoral Fellow**, Advisor: Dr. Ignacio Franco
Department of Chemistry & Department of Physics, University of Rochester, NY

2011-2016 **Research Assistant**, Advisor: Dr. Sophya V. Garashchuk
Department of Chemistry and Biochemistry, University of South Carolina-Columbia, SC

2010-2011 **Research Assistant**, Advisor: Dr. Qunxiang Li
Department of Chemical Physics, University of Science and Technology of China, Hefei, China

Education

2011-2016 PhD in Theoretical Chemistry, University of South Carolina (USC)
Dissertation: Estimation of Quantum Effects of Nuclei in Large Molecular Systems

2007-2011 BSc in Chemical Physics, University of Science and Technology of China (USTC)
Thesis: The Spin-Polarization Transport Properties of the $M@Au_6$ (M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni) Clusters Using *ab initio* Methods.

Honors & Awards

2022 71st Lindau Nobel Laureate Meeting, Lindau, Germany
2020 Pacific Conference on Spectroscopy and Dynamics Scholarship
2018 Young Investigator Award, ACS, Division of Physical Chemistry
2018 Young Investigator Travel Award, APS, Division of Chemical Physics
2015 Dr. James R. Durig Graduate Student Travel Award, USC
2014 $SICM^2$ Parallel Computing Workshop, Stony Brook University, Institute of Advanced Material Science
2011 Outstanding Student Scholarship, Department of Chemical Physics, USTC
2005 Chinese Chemistry Olympiad, Jiangsu Jingjiang Senior High School, Jiangsu, China

Service & Professional Membership

2022 Session Chair of TSRC **Quantum Frontiers in Molecular Science**
Since 2022 Advisory Board of *Molecules*
Since 2016 Peer Reviewer for *Sci. Adv., J. Phys. Chem. Lett., J. Chem. Phys., J. Phys. Chem., Chem. Sci., Phys. Rev., Sci. Rep., ACS Nano, Entropy, Molecules*
2018 Volunteer for the *Contact Congress Booth* in APS, Los Angeles, CA
Since 2018 Member of UAW Local 5810
2014 Judge for the *USC Science Fair of Midlands Region*, Columbia, SC

Since 2014 Members of the American Physical Society (APS), the American Chemical Society (ACS), The Optical Society of America

Invited Talks

Jul 2023 **TSRC Polariton Chemistry and Molecular Cavity Quantum Electrodynamics,** Telluride, CO, USA
Collective polariton chemistry under strong light-matter coupling

2022 **TSRC Quantum Frontiers in Molecular Science**
Control of quantum interference in molecular two-photon-absorption by entangled light

2021 **PACIFICHEM**, Honolulu, Hawaii, USA
B. Gu and S. Mukamel, Cavity photochemistry: Controlling Conical Intersection Dynamics by Cavity Polaritons

2021 **Fall ACS National Meeting,** Atlanta, GA
B. Gu and S. Mukamel, "Molecular Polaritons from Infrared to X-ray: Dynamics and Spectroscopy"

2020 **Ultrafast Processes in Atoms, Molecules, and Nanosystems,** Virtual Conference
B. Gu and S. Mukamel, "Manipulating Ultrafast Conical Intersection Dynamics by Optical Cavities"

2020 **Polariton Chemistry Webinar,** Virtual Conference
B. Gu and S. Mukamel, "Cavity Photochemistry: Dynamics and Spectroscopy"

2018 **ACS National Meeting**, Boston, MA
B. Gu and I. Franco, "Quantifying Early-Time Quantum Decoherence Dynamics through Fluctuations"

Contributed Talks

2021 **International Conference on Time Resolved Vibrational Spectroscopy (TRVS), Early Career Symposium,** Virtual Conference
B. Gu and S. Mukamel, Time-resolved spectroscopy for photochemistry in optical cavities

2020 **22nd International Conference on Ultrafast Phenomena**, Shanghai, China
B. Gu and S. Mukamel, "Manipulating Ultrafast Conical Intersection Dynamics by Optical Cavities"

2020 **OSA Frontiers in Optics + Laser Science APS/DLS,** Virtual Conference
B. Gu and S. Mukamel, "Manipulating Two-Photon Absorption of Cavity Polaritons by Entangled Light"

2020 **67th Pacific Conference on Spectroscopy and Dynamics,** San Diego, CA
B. Gu and S. Mukamel, "Manipulating conical intersection dynamics by optical cavities"

2018 **APS National Meeting**, Los Angeles, CA
R. Carey, L. Chen, B. Gu, I. Franco, "When can time-dependent currents be reproduced by the Landauer steady-state approximation?"

2018 **APS National Meeting**, Los Angeles, CA
B. Gu, I. Franco, "Partial hydrodynamic representation of quantum molecular dynamics"

2018 **APS National Meeting**, Los Angeles, CA
B. Gu, A. Garzon, I. Franco, "Optical absorption properties of laser-dressed matter"

2018 **APS National Meeting**, Los Angeles, CA
B. Gu, I. Franco "Quantifying early-time quantum decoherence through fluctuations"

2017 **Center for Coherence and Quantum Optics**, University of Rochester
B. Gu, I. Franco, “Optical absorption of laser-dressed materials”

2015 **Physical Chemistry Divisional Seminar**, University of South Carolina
B. Gu, V. Rassolov, S. Garashchuk, “Quantum molecular dynamics with friction: Application to solid helium”

2014 **81st Annual Meeting of the APS Southeastern Section**, Columbia, SC
B. Gu, V. Rassolov, S. Garashchuk, “Estimation of quantum effects of atomic solids using quantum trajectory dynamics with dissipation”

2012 **Physical Chemistry Divisional Seminar**, University of South Carolina
B. Gu, S. Garashchuk, “The zero-point energy leak in molecular dynamics”

Publications

Peer-reviewed journals (*Corresponding author)

36 **B. Gu*,** S. Sun, F. Chen, S. Mukamel, Photoelectron spectroscopy with entangled photons: enhanced temporal and spectral resolution, to appear in PNAS, **2023**

35 H Yong, S Sun, **B Gu**, S Mukamel, Attosecond Charge Migration in Molecules Imaged by Combined X-ray and Electron Diffraction, *J. Am. Chem. Soc*. **2022**, 144, 45, 20710–20716

34 Y Nam, D Cho, **B Gu**, JR Rouxel, D Keefer, N Govind, S. Mukamel, Time-Evolving Chirality Loss in Molecular Photodissociation Monitored by X-ray Circular Dichroism Spectroscopy, *J. Am. Chem. Soc.* **2022**, 144, 44, 20400-20410

33 F. Chen, **B. Gu**, S. Mukamel, Monitoring Conical Intersection Dynamics by Entangled Two-Photon Absorption, *ACS Photonics,* **2022**, 9, 6, 1889–1894

32 D. Cho, **B. Gu***, S. Mukamel, Multidimensional Spectroscopy of Polaritonic Conical Intersections in an Optical Cavity, J. Am. Chem. Soc. **2022,** 144, 17, 7758–7767

31 **B. Gu**, D. Keefer, F. Aleotti, A. Nenov, M. Gavavelli, S. Mukamel, Photoisomerization Transition State Manipulation by Entangled-Two-Photon-Absorption, *Proc. Natl. Acad. Sci. U.S.A*, 2021, 118 (47) e2116868118

30 **B. Gu*,** D. Keefer, and S. Mukamel, Wavepacket Control and Simulation Protocols for Entangled Two-Photon-Absorption of Molecules, J. Chem. Theory. Comput., 2021, 18, 1, 406–414

29 S. Sun, **B. Gu,** S. Mukamel, Polariton Ring Current and Circular Dichroism Signals in Mg-porphyrin, *Chem. Sci.,* **2022**, DOI: 10.1039/D1SC04341B

28 **B. Gu*** and S. Mukamel, Photon Correlation Signals of Entangled-Photon-Excited Coupled-Cavity Polaritons, *ACS Photonics*, **2022**

27 **B. Gu**, S. M. Cavaletto, D. R. Nascimento, M. Khalil, N. Govind, and S. Mukamel, Manipulating Valence and Core Electronic Excitations of a Transition-Metal Complex Using UV/Vis and X-ray Cavities, *Chem. Sci.,* **2021,** 12, 8088-8095

26 A. Eshun, **B. Gu**, Oleg Varnavski, S. Asban, K. E. Dorfman, S. Mukamel, T. Goodson III, Investigations of Molecular Optical Properties Using Quantum Light and HOM Interferometry, *J. Am. Chem. Soc.,* **2021**, 143, 9070-9081

25 **B. Gu*** and S. Mukamel, Optical-Cavity Manipulation of Conical Intersections and Singlet Fission in Pentacene Dimers, *J. Phys. Chem. Lett.,* **2021**, 12, 2052-2056

24 K. E. Dorfman, S. Asban, **B. Gu**, and S. Mukamel, Hong-Ou-Mandel interferometry and spectroscopy using entangled photons, *Communications Physics*, **2021,** 4, 1-7

23 **Gu, B.,** Nenov, A., Segatta, F., Garavelli, M. & Mukamel, S. Manipulating Core Excitations in Molecules by X-Ray Cavities. *Phys. Rev. Lett.* **2021**, 126, 053201

22 D. Keefer, F. Aleotti, J. Rouxel, F. Segatta, **B. Gu,** A. Nenov, M. Garavelli, and S. Mukamel, Imaging Conical Intersection Dynamics during Azobenzene Photoisomerization by Ultrafast X-Ray Diffraction, *Proc. Natl. Acad. Sci. U.S.A*, **2021,** 118, e2022037118

21 **B. Gu*** and S. Mukamel, Manipulating Two-Photon-Absorption of Cavity Polaritons by Entangled Light, *J. Phys. Chem. Lett.,* **2020,** 11, 8177–8182

20 **B. Gu*** and S. Mukamel, Cooperative conical intersection dynamics of two pyrazine molecules strongly coupled to an optical cavity, *J. Phys. Chem. Lett.* **2020,** 11, 5555-5562

19 W. Hu, **B. Gu** and I. Franco, Toward the laser control of electronic decoherence, *J. Chem. Phys.*, **2020,** 152, 184305

18 **B. Gu*** and S. Mukamel, "Manipulating nonadiabatic conical intersection dynamics by optical cavities", *Chem. Sci.,* **2020**, 11, 1290-1298

17 **B. Gu*,** "Diagrammatic time-local master equation for open quantum systems", *Phys. Rev. A*, **2020,** 101, 012121

16 **B. Gu** and I. Franco, "When can quantum decoherence be mimicked through classical noise" *J. Chem. Phys.* **2019**, 151, 014109

15 **B. Gu** and I. Franco, "Electronic interactions do not affect electronic decoherence in the pure-dephasing limit", *J. Chem. Phys.* **2018**, 149, 174115

14 **B. Gu** and I. Franco, "Optical Absorption Properties of Laser-Dressed Matter" *Phys. Rev. A* **2018**, 98, 063412

13 W. Hu, **B. Gu**, I. Franco, "Lessons on electronic decoherence in molecules from exact modeling*", J. Chem. Phys.* **2018**, 148, 134304

12 **B. Gu**, I. Franco, "Generalized theory of the timescale of molecular electronic decoherence in condensed phase", *J. Phys. Chem. Lett.* **2018**, 9, 773−778

11 **Gu, B.;** Franco, I. Quantifying Early-Time Quantum Decoherence Dynamics through Fluctuations. *J. Phys. Chem. Lett.* **2017**, *8*, 4289–4294

10 **B. Gu*** and I. Franco, "Partial hydrodynamic representation of quantum molecular dynamics" *J. Chem. Phys.* **2017**, 146, 194104

9 R. Carey, L. Chen, **B. Gu** and I. Franco, "When can time-dependent currents be reproduced by the Landauer steady-state approximation?" *J. Chem. Phys.* **2017**, 146, 174101

8 I. Savchenko, **B. Gu**, T. Heine, S. Garashchuk and J. Jakowski, "Nuclear quantum effects on adsorption of H_2 and isotopologues on metal ions", *Chem. Phys. Lett.* **2017**, 670, 64-70

7 B. Som, S. R. Salpage, J. Son, **B. Gu**, S. G. Karakalos, M. D. Smith and L. S. Shimizu, "Pillars of assembled pyridyl bis-urea macrocycles: A robust synthon to organize diiodotetrafluorobenzenes" *CrystEngComm* **2017**, 19, 484-491

6 **B. Gu** and S. Garashchuk, "Quantum dynamics with Gaussian bases defined by the quantum trajectories", *J. Phys. Chem. A* **2016**, 120, 3023-3031

5 **B. Gu**, V. Rassolov and S. Garashchuk, “Symmetrization of the nuclear wavefunctions defined by the quantum trajectory dynamics”, *Theor. Chem. Acc.* **2016**, 135, 267

4 **B. Gu** and S. Garashchuk, “Determination of the collective modes from the quantum-mechanical time-correlation functions”, *Theor. Chem. Acc.* **2015**, 134, 129

3 **B. Gu**, R. J. Hinde, V. Rassolov and S. Garashchuk, “Estimation of quantum mechanical effects of atomic solids with quantum trajectory method with dissipation*”, J. Chem. Theory Comput.* **2015**, 11, 2891-2899

2 S. Garashchuk, **B. Gu** and J. Mazzuca, “Calculation of the quantum-mechanical tunneling in bound potentials” *J. Theory Chem.* **2014**, 2014, 240491

1 S. Garashchuk, V. Dixit, **B. Gu** and J. Mazzuca, “The Schrodinger equation with friction from the quantum trajectory perspective”, *J. Chem. Phys.* **2013**, 138, 054107

Conference proceedings

1 **B. Gu** and S. Garashchuk, “Molecular dynamics of large systems with quantum corrections for the nuclei” *AIP Conf. Proc.* **2015**, 1702, 090014