David B. Lingerfelt

Curriculum Vitae

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Education and Training

2012–2017 **PhD**, *Univ. of Washington*, Seattle, WA.
Physical Chemistry. Conferred June, 2017
Dissertation: "Excited State Molecular Dynamics: Beyond the Born-Oppenheimer Approximation"

2005–2010 **BS**, *Univ. of North Carolina Asheville*, Asheville, NC.
Chemistry major. Mathematics minor. Distinction in Chemistry. University Research Scholar.

Professional Experience

2021–current **R&D Associate**, *Nanomaterials Theory Institute*, Center for Nanophase Materials Sciences, Oak Ridge National Lab.

2018–2021 **Postdoctoral Researcher**, *Nanomaterials Theory Institute*, Center for Nanophase Materials Sciences, Oak Ridge National Lab.
Supervisors: Panchapakesan Ganesh (Group Leader), Bobby Sumpter (Section Head)

2017–2018 **Postdoctoral Researcher**, *Chemistry Dept., Univ. of Washington*, Seattle, WA.
Supervisor: Xiaosong Li

2017 **Lecturer**, *Chemistry Dept., Univ. of Washington*, Seattle, WA.

Awards

- Center for Nanophase Materials Sciences, Postdoctoral Researcher Award, 2020
- Clean Energy Institute Travel Award (for contributed talk at Pacifichem 2015)
- Clean Energy Institute Graduate Fellowship, 2015
- Graduate Student Merit Fellowship, Univ. of Washington, 2014-2015
- Benton Seymour Rabinovitch Endowed Fellowship, Univ. of Washington, 2012
- Outstanding Performance in Physical Chemistry, Univ. of North Carolina Asheville, 2008-2009
- NASA North Carolina Space Grant, 2008

Synergistic and Outreach Activities

- Reviewer for *Scientific Reports*, an open access Nature Publishing Group journal.
- ORNL HERE post-baccalaureate researcher mentor, Feb-May 2020.
- Founding member of Univ. of Washington High Performance Computing Club, 2015
- Undergraduate research mentor, Amgen Scholars program, Summer 2013 & 2014.

Publications (* denotes shared first authorship)

2022:

DBL, A. Yoshimura, J. Jakowski, P. Ganesh, and B. G. Sumpter, "Extracting Inelastic Scattering Cross Sections for Finite and Aperiodic Materials from Electronic Dynamics Simulations" (submitted)

A. Yoshimura, M. Lamparski, J. Giedt, **DBL**, J. Jakowski, P. Ganesh, T. Yu, B. Sumpter, V. Meunier, "Quantum Theory of Electronic Excitation and Sputtering by Transmission Electron Microscopy" *Nanoscale*, (Advance Article)

O. Dyck, F. Bao, M. Ziatdinov, A. Yousefzadi Nobakht, K. Law, A. Maksov, B. G. Sumpter, R. Archibald, S. Jesse, S. V. Kalinin, and **DBL**, "Strain-Induced Asymmetry and On-Site Dynamics of Silicon Defects in Graphene", *Carbon Trends*, 9, 100189

DBL, P. Ganesh, B. G. Sumpter, and J. Jakowski, "From Ground to Excited Electronic State Dynamics of Electron and Ion Irradiated Graphene Nanomaterials", in *Properties and Functionalization of Graphene: A Computational Chemistry Approach*, Theoretical and Computational Chemistry (book series) Volume 21, Edited by Dinadayalane Tandabany & Frank Hagelberg, 87–107

2021:

DBL, T. Yu, A. Yoshimura, J. Jakowski, P. Ganesh, B. G. Sumpter, "Nonadiabatic Effects on Defect Diffusion in Silicon-Doped Nanographenes" *Nano Lett.* 21 (1), 236–242

T. Yu, **DBL**, J. Jakowski, P. Ganesh, B. G. Sumpter, "Electron-Beam Induced Molecular Plasmon Excitation and Energy Transfer in Silver Molecular Nanowires" *J. Phys. Chem. A* 125 (1), 74–87

2020:

A. Y. Nobakht, O. Dyck, **DBL**, F. Bao, M. Ziatdinov, A. Maksov, B. G. Sumpter, R. Archibald, S. Jesse, S. V. Kalinin, K. J. H. Law, "Reconstruction of Effective Potential from Statistical Analysis of Dynamic Trajectories", *AIP Adv.* 10, 065034

G. U. Kuda-Singappulige, A. Wildman, **DBL**, X. Li, C. Aikens, "Ultrafast Nonradiative Decay of a Dipolar Plasmon-like State in Naphthalene" *J. Phys. Chem. A* 124 (47), 9729–9737

O. A. Hull, **DBL**, X. Li, C. M. Aikens, "Electronic Structure and Nonadiabatic Dynamics of Atomic Silver Nanowire–N_2 Systems" *J. Phys. Chem. C* 124 (38), 20834-20845

G. U. Kuda-Singappulige, **DBL**, X. Li, C. M. Aikens, "Ultrafast Nonlinear Plasmon Decay Processes in Silver Nanoclusters" *J. Phys. Chem. C* 124 (37), 20477-20487

O. Dyck, **DBL**, S. Kim, S. Jesse, S. V. Kalinin, "Direct Matter Disassembly *via* Electron Beam Control: Electron-Beam-Mediated Catalytic Etching of Graphene by Nanoparticles" *Nanotechnology* 31 (24), 245303

DBL, P. Ganesh, J. Jakowski, B. G. Sumpter, "Understanding Beam Induced Electronic Excitations in Materials", *J. Chem. Theory Comput.* 16, 1200–1214.

2019:

S. V. Kalinin, O. Dyck, N. Balke, S. Neumayer, W. Tsai, R. Vasudevan, **DBL**, M. Ahmadi, M. Ziatdinov, M. T. McDowell, E. Strelcov, "Toward Electrochemical Studies on the Nanometer and Atomic Scales: Progress, Challenges, and Opportunities" *ACS Nano*, 2019, 13, 9735–9780.

DBL, J. Jakowski, P. Ganesh, B. Sumpter, "A TD-DFT Treatment of Electronic Excitations in the STEM Spanning Dipole and Impact Scattering Regimes" *Microsc. Microanal.*, 2019, 25, 2300–2301.

O. Dyck, M. Ziatdinov, **DBL**, R. R. Unocic, B. M. Hudak, A. R. Lupini, S. Jesse, S. V Kalinin, "Atom-by-Atom Fabrication with Electron Beams" *Nat. Rev. Mater.*, 2019, 4, 497–507.

DBL, P. Ganesh, J. Jakowski, B. G. Sumpter, "Electronically Nonadiabatic Structural Transformations Promoted by Electron Beams" *Adv. Funct. Mater.*, 2019, 29, 1901901.

R. D. Senanayake, **DBL**, G.U. Kuda-Singappulige, X. Li, C. M. Aikens, "Real-Time TDDFT Investigation of Optical Absorption in Gold Nanowires" *J. Phys. Chem. C*, 2019, 123, 14734–14745.

T. F. Stetina, S. Sun, **DBL**, A. Clark, X. Li, "The Role of Excited-State Proton Relays in the Photochemical Dynamics of Water Nanodroplets" *J. Phys. Chem. Lett.*, 2019, 10, 3694–3698.

2018:

G. Donati, **DBL**, C. M. Aikens, X. Li, "Anisotropic Polarizability-Induced Plasmon Transfer" *J. Phys. Chem. C*, 2018, 122, 10621–10626.

*J. J. Radler, ***DBL**, F. N. Castellano, L. X. Chen, X. Li, "Role of Vibrational Dynamics on Excited-State Electronic Coherence in a Binuclear Platinum Complex" *J. Phys. Chem. A*, 2018, 122, 5071–5077.

2017:

H. Liu, C. K. Brozek, S. Sun, **DBL**, D. R. Gamelin, X. Li, "A Hybrid Quantum-Classical Model of Electrostatics in Multiply Charged Quantum Dots" *J. Phys. Chem. C*, 2017, 121, 26086–26095.

G. Donati, A. Wildman, S. Caprasecca, **DBL**, F. Lipparini, B. Mennucci, X. Li, "Coupling Real-Time Time-Dependent Density Functional Theory with Polarizable Force Field" *J. Phys. Chem. Lett.*, 2017, 8, 5283–5289.

G. Donati, **DBL**, C. Aikens, X. Li,"Molecular Vibration Induced Plasmon Decay" *J. Phys. Chem. C*, 2017, 121, 15368–15374.

A. Petrone, D. B. Williams-Young, **DBL**, X. Li, "*Ab Initio* Excited State Transient Raman Analysis" *J. Phys. Chem. A*, 2017, 121, 3958–3965.

DBL, P. J. Lestrange, J. J. Radler, S. E. Brown-Xu, P. Kim, F. N. Castellano, L. X. Chen, X. Li, "Can Excited State Electronic Coherence be Tuned via Molecular Structural Modification? A First-Principles Quantum Electronic Dynamics Study of Pyrazolate-Bridged Pt(II) Dimers", *J. Phys. Chem. A*, 2017, 121, 1932–1939

2016:

*J. J. Goings, ***DBL**, X. Li, "Can Quantized Vibrational Effects be Obtained from Ehrenfest Mixed Quantum-Classical Dynamics?", *J. Phys. Chem. Lett.*, 2016, 7, 5193–5197.

A. Petrone, **DBL**, D. B. Williams-Young, X. Li, "*Ab Initio* Transient Vibrational Spectral Analysis", *J. Phys. Chem. Lett.*, 2016, 7, 4501.

G. Donati, **DBL**, A. Petrone, N. Rega, X. Li, "Watching Polaron Pair Formation from First-Principles Electron-Nuclear Dynamics", *J. Phys. Chem. A*, 2016, 120, 7255–7261.

*E. Q. Chong, ***DBL**, *A. Petrone, X. Li, "Classical or Quantum? A Computational Study of Small Ion Diffusion in II-VI Semiconductor Quantum Dots", *J. Phys. Chem. C*, 2016, 120, 19434.

DBL, D. B. Williams-Young, A. Petrone, X. Li, "Direct *ab Initio* (Meta-)Surface-Hopping Dynamics", *J. Chem. Theory Comput.*, 2016, 12, 935–945.

2015:

F. Ding, J. J. Goings, H. Liu, **DBL**, X. Li, "*Ab Initio* Two-component Ehrenfest Dynamics", *J. Chem. Phys.*, 2015, 143, 114105.

B. Peng, **DBL**, F. Ding, C. Aikens, X. Li, "Real-Time TDDFT Studies of Exciton Decay and Transfer in Silver Nanowire Arrays", *J. Phys. Chem. C*, 2015, 119, 6421.

F. Ding, **DBL**, B. Mennucci, X. Li, "Time-Dependent Non-equilibrium Dielectric Response in QM/Continuum Approaches", *J. Chem. Phys.*, 2015, 142, 034120.

2014:

A. Petrone, **DBL**, N. Rega, X. Li, "From Charge-Transfer to Charge-Separated State: A Perspective from the Real-Time TDDFT Excitonic Dynamics", *Phys. Chem. Chem. Phys.*, 2014, 16, 24457.

S. A. Fischer, **DBL**, J. W. May, X. Li, "Non-adiabatic Molecular Dynamics Investigation of Photoionization State Formation and Lifetime in Mn^{2+}-Doped ZnO Quantum Dots", *Phys. Chem. Chem. Phys.*, 2014, 16, 17507.

DBL, S. A. Fischer, J. W. May, X. Li, "Dynamical Investigations of Inhomogeneous Vibrational Broadening in Diluted Magnetic Semiconductor Nanocrystals", *J. Phys. Chem. C*, 2014, 118, 3266–3273.

Presentations

Invited Talks:

"Understanding and Controlling Materials Atom-by-Atom," 2022 MRS Spring Meeting, May 23, 2022. Honolulu, HI

"Matter-Beam Interactions: Photochemistry with Virtual Photons", Departmental Seminar, Tennessee Technical University Chemistry Department, Nov. 9, 2019. Cookeville, TN.

"Electronic Excitations from Electron Beam Irradiation and Their Role in Atomic Scale Material Manipulations", Workshop on Atom by Atom Fabrication Via Electron Beams and Scanning Probes, Nov. 1-2, 2018. Oak Ridge, Tennessee.

Contributed Talks:

"First-Principles Methods for Simulating Inelastic Scattering of High Energy Electron Beams by Materials", APS March Meeting, March 17, 2022, Chicago, IL.

"Matter-Beam Interactions: Photochemistry with Virtual Photons?", APS March Meeting, March 2, 2020, Denver, CO (canceled due to COVID-19 pandemic; slides shared in lieu of presentation)

"A TD-DFT Method for the Prediction of Electronic Response to Electron Beam Irradiation", Southeastern Theoretical Chemistry Association Meeting May 17, 2019, Knoxville, TN.

"Time Dependent Self Consistent Field Methods for Simulating Electron Beam – Materials Interactions ", Oak Ridge Postdoc Association Research Symposium, Aug. 7, 2018. Oak Ridge, TN.

"Charge Carrier Lifetimes in $Mn_xZn_{1-x}O$ Nanocrystals from Non-Adiabatic Molecular Dynamics Simulations", International Chemical Congress of Pacific Basin Societies (Pacifichem) Dec. 15-20, 2015. Honolulu, HI.

Contributed Posters:

"Excited State Silicon Defect Diffusion Pathways in Graphene Nanomaterials", Center For Nanophase Materials Sciences, Annual User meeting, Aug. 10-12 2020 (held virtually due to COVID-19 pandemic)

"A Time-Dependent Electronic Structure Theory Route to Predicting Electronic Excitations Induced through Inelastic Electron Scattering", Frontiers of Electron Microscopy and Materials Science, Sept. 1-6 2019. Asheville, NC.

"A TD-DFT Treatment of Electronic Excitations in the STEM Spanning Dipole and Impact Scattering Regimes", Microscopy and Microanalyis Meeting, Aug. 4-8, 2019. Portland, OR.

"Small Cation Diffusion in II-VI Semiconductor Nanocrystals: Resolving Vibrational Energy Eigenstate Delocalization Trends", Electronic Structure and Processes at Molecular-Based Interfaces 8. Oct. 13-16, 2015. Oracle, AZ.

"Mechanisms of Exciton Diffusion and Dissociation in Organic Photovoltaic Materials: Are Electrons or Holes the Most Mobile Charge Carriers?" 248th ACS National Meeting, Poster PHYS-474, Aug. 10-14, 2014. San Francisco, CA.