

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.
Thesis: “On the Relation of Alkyl Chain Length to Dehydrogenation Energy for Primary Alcohols on a Catalytic Rhodium Surface: A Periodic DFT Study”
- 2013 **Certificate**, *European Summerschool in Quantum Chemistry*, Sicily, Italy.

Professional Experience

- 2018–Current **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.
Courses Taught:
○ (Summer 2017) Chem110: Preparation for General Chemistry
○ (Autumn 2017) Chem120: Principles of Chemistry I
- 2010–2011 **Chromatography Technician**, *SECON of New England*, Worcester, MA.

Research Activities

Method Development • Excited state electronic structure via response theory formalism and explicitly time-dependent electronic dynamics • First principles treatment (in both real-space and k -space) of electronic and vibrational excitation cross sections for materials perturbed by beams of swift charged particles • Mixed quantum-classical, electronically nonadiabatic molecular dynamics approaches for far-from-equilibrium systems • Leveraging machine learning techniques to prevent redundant calculations in statistically-significant ensembles of molecular and materials simulations.

Scientific Applications • Study the effects of structural and compositional impurities — as well as finite-size and edge-induced effects — on emergent quantum phenomena in nanoscale materials • Simulate materials responses to spatially inhomogeneous scalar (electric) and vector (magnetic) potentials • Identify excited state pathways relevant to reactions induced under electron and ion beam irradiation. • Resolve topological character of material’s electronic structure in exotic phases (quantum anomalous hall, etc.).

Theory-Experiment Symbiosis • Work closely with experimental colleagues in electron/ion microscopy/spectroscopy to interpret and explain novel experimental results. • Identify target experiments that can both validate theoretical approaches and guide future directions for empirical studies.

Awards

- Center for Nanophase Materials Sciences, Postdoctoral Researcher Award, 2020
- Clean Energy Institute Graduate Fellowship, 2015
- Clean Energy Institute Travel Award (for contributed talk at Pacifichem 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

Professional Society Memberships

- o American Physical Society, Member

Synergistic and Outreach Activities

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

Publications

(* denotes shared first authorship)

2020:

O. Dyck*, **DBL***, F. Bao, M. Ziatdinov, A. Yousefzadi Nobakht, S. Shin, K. Law, A. Maksov, B. G. Sumpter, R. Archibald, S. Jesse, and S. V. Kalinin, "Strain-Induced Asymmetry and On-Site Dynamics of Atomic Impurities in Graphene" (submitted)

DBL, T. Yu, A. Yoshimura, J. Jakowski, P. Ganesh, B. G. Sumpter, "Nonadiabatic Effects on Defect Diffusion in Silicon-Doped Nanographenes" (in review)

T. Yu, **DBL**, J. Jakowski, P. Ganesh, B. G. Sumpter, "Electron-Beam Induced Molecular Plasmon Excitation and Energy Transfer in Silver Molecular Nanowires" (in review)

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*, Elsevier (accepted; schedule for printing 2021)

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* (just accepted)

O. A. Hull, **DBL**, X. Li, C. M. Aikens, "Electronic Structure and Nonadiabatic Dynamics of Atomic Silver Nanowire-N₂ 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. Lestrangle, 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 Mn²⁺-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:

"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.

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

Contributed Talks:

"A TD-DFT Method for the Prediction of Electronic Response to Electron Beam Irradiation", Southeastern Theoretical Chemistry Association Meeting May 16-18, 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 Microanalysis 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.