Galen T. Craven

Theoretical Division, Los Alamos National Laboratory

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Professional Experience

Scientist, Theoretical Division, Los Alamos National Laboratory, 2020 - *current*

Director's Postdoctoral Fellow, Los Alamos National Laboratory, 2019 - 2020
Physics and Chemistry of Materials Group

Postdoctoral Researcher, University of Pennsylvania, 2015 - 2019
Department of Chemistry Advisor: Abraham Nitzan

Education

Ph.D., Georgia Institute of Technology, 2014
Chemistry Advisor: Rigoberto Hernandez

B.S., University of North Alabama, 2009
Chemistry

Academic Awards

Los Alamos National Laboratory

- Director's Postdoctoral Fellowship *2019*
- Center for Nonlinear Studies (CNLS) Fellowship *2019*

University of Pennsylvania

- ACS PHYS Division Young Investigator Award *2017*
- Peter Salamon Award for Young Scientists, Telluride Science Research Center *2016*

Georgia Institute of Technology

- Georgia Tech Research and Innovation Conference Award Winner *2014*
- William Henry Emerson Fellowship *2009*

University of North Alabama

- M. M. Striplin Jr. Endowed Scholarship *2009*

Research Highlights

G. T. Craven and A. Nitzan
"Wiedemann-Franz law for molecular hopping transport"
Nano Lett. 20, 989 (2020)

G. T. Craven, Dahai He, and A. Nitzan
"Electron-transfer-induced thermal and thermoelectric rectification"
Phys. Rev. Lett. 121, 247704 (2018)

G. T. Craven and A. Nitzan
"Electrothermal transistor effect and cyclic electronic currents in multithermal charge transfer networks"
Phys. Rev. Lett. 118, 207201 (2017)

G. T. Craven and A. Nitzan
"Electron transfer across a thermal gradient"
Proc. Natl. Acad. Sci. 113, 9421 (2016)

G. T. Craven and R. Hernandez
"Lagrangian descriptors of thermalized transition states on time-varying energy surfaces"
Phys. Rev. Lett. 115, 148301 (2015)

Complete Publications List

[35] E. Shinkle, A. Pachalieva, S. Matin, **G. T. Craven**, N. Lubbers
"Thermodynamic transferability in coarse-grained force fields using graph neural networks"
In preparation

[34] R. Chen and **G. T. Craven**
"The effect of temperature oscillations on energy storage rectification in harmonic systems"
Invited article for "Focus Issue on Energy Conversion Physics of Molecular Scale Junctions"
Submitted to *J. Phys. Condens. Matter*

[33] M. Anjum, T. Gibson, **G. T. Craven**, S. Tretiak, A. Abdelkefil
"Multiphysics analysis of mechanical responses in micro-reactors under varied operating conditions"
Submitted to *Eur. J. Mech. A, Solids*

[32] A. J. White, **G. T. Craven**, V. Sharma, L. A. Collins
"Optical and transport properties of plasma mixtures from *ab initio* molecular dynamics"
Submitted to *Phys. Plasmas*

[31] L. Johnson, W. Malone, J. Rizk, R. Chen, T. Gibson, M.W.D. Cooper, **G. T. Craven**
"Machine learning method to determine concentrations of structural defects in irradiated materials"
Submitted to *Comput. Mater. Sci.*

[30] R. Chen, T. Gibson, **G. T. Craven**
"Molecular heat transport across a time-periodic temperature gradient"
Submitted to *J. Chem. Phys.*

[29] **G. T. Craven**, R. Chen, M.W.D. Cooper, C. Matthews, J. Rizk, W. Malone, L. Johnson, T. Gibson, and D. A. Andersson
"Data-driven methods for diffusivity prediction in nuclear fuels"
Comput. Mater. Sci. 230, 112442 (2023)

[28] R. Chen, T. Gibson, **G. T. Craven**
"Energy transport between heat baths with oscillating temperatures"
Phys. Rev. E 108, 024148 (2023)

[27] M.W.D. Cooper, J. Rizk, C. Matthews, **G. T. Craven**, T. Gibson, D. A. Andersson
"Simulations of self- and Xe diffusivity in uranium mononitride including chemistry and irradiation effects"
J. Nucl. Mater. 587, 154685 (2023)

[26] **G. T. Craven** and A. Nitzan
"Electron hopping heat transport in molecules"
J. Chem. Phys. 158, 174306 (2023)

[25] B. Cui, **G. T. Craven**, and A. Nitzan
"Heat transport induced by electron transfer: A general temperature quantum calculation"
J. Chem. Phys. 155, 194104 (2021)

[24] **G. T. Craven**, N. Lubbers, K. Barros, and S. Tretiak
"Machine learning approaches for structural and thermodynamic properties of a Lennard-Jones fluid"
J. Chem. Phys. 153, 104502 (2020)

[23] **G. T. Craven**, N. Lubbers, K. Barros, and S. Tretiak
"*Ex machina* determination of structural correlation functions"
J. Phys. Chem. Lett. 11, 4372 (2020)

[22] **G. T. Craven** and A. Nitzan
"Wiedemann-Franz law for molecular hopping transport"
Nano Lett. 20, 989 (2020)

Complete Publications List continued

[21] **G. T. Craven**, D. He, and A. Nitzan
"Electron-transfer-induced thermal and thermoelectric rectification"
Phys. Rev. Lett. 121, 247704 (2018)

[20] **G. T. Craven**, R. Chen, and A. Nitzan
"Upside/Downside statistical mechanics of nonequilibrium Brownian motion. II. Heat transfer and energy partitioning of a free particle"
J. Chem. Phys. 149, 104103 (2018)

[19] **G. T. Craven** and A. Nitzan
"Upside/Downside statistical mechanics of nonequilibrium Brownian motion. I. Distributions, moments, and correlation functions of a free particle"
J. Chem. Phys. 148, 044101 (2018)

[18] R. Chen, **G. T. Craven**, and A. Nitzan
"Electron-transfer-induced and phononic heat transport in molecular environments"
— Selected as an AIP Scilights article —
J. Chem. Phys. 147, 124101 (2017)

[17] **G. T. Craven**, A. Junginger, and R. Hernandez
"Lagrangian descriptors of driven chemical reaction manifolds"
Phys. Rev. E 96, 022222 (2017)

[16] F. Revuelta, **G. T. Craven**, T. Bartsch, F. Borondo, R. M. Benito, and R. Hernandez
"Transition state theory for activated systems with driven anharmonic barriers"
J. Chem. Phys. 147, 074104 (2017)

[15] **G. T. Craven** and A. Nitzan
"Electrothermal transistor effect and cyclic electronic currents in multithermal charge transfer networks"
Phys. Rev. Lett. 118, 207201 (2017)

[14] **G. T. Craven** and A. Nitzan
"Electron transfer at thermally heterogeneous molecule-metal interfaces"
— In the themed issue on "Frontiers in Molecular Scale Electronics" —
J. Chem. Phys. 146, 092305 (2017)

[13] **G. T. Craven** and A. Nitzan
"Electron transfer across a thermal gradient"
Proc. Natl. Acad. Sci. 113, 9421 (2016)

[12] A. Junginger, **G. T. Craven**, T. Bartsch, F. Revuelta, F. Borondo, R. M. Benito, and R. Hernandez
"Transition state geometry of thermal chemical reactions on time-dependent double-well potentials"
— In the themed issue on "Insights from Advanced Methods in Molecular Dynamics" —
Phys. Chem. Chem. Phys. 18, 30270 (2016)

[11] **G. T. Craven** and R. Hernandez
"Deconstructing field-induced ketene isomerization through Lagrangian descriptors"
Phys. Chem. Chem. Phys. 18, 4008 (2016)

[10] A. V. Popov, **G. T. Craven**, and R. Hernandez
"Nonequilibrium structure in sequential assembly"
Phys. Rev. E 92, 052108 (2015)

[9] **G. T. Craven** and R. Hernandez
"Lagrangian descriptors of thermalized transition states on time-varying energy surfaces"
Phys. Rev. Lett. 115, 148301 (2015)

Complete Publications List continued

[8] **G. T. Craven**, A. V. Popov, and R. Hernandez
"Stochastic dynamics of penetrable rods in one dimension: Entangled dynamics and transport properties"
J. Chem. Phys. 142, 154906 (2015)

[7] **G. T. Craven**, T. Bartsch, and R. Hernandez
"Chemical reactions induced by oscillating external fields in weak thermal environments"
J. Chem. Phys. 142, 074108 (2015)

[6] **G. T. Craven**, A. V. Popov, and R. Hernandez
"Effective surface coverage of coarse-grained soft matter"
J. Phys. Chem. B 118, 14092 (2014)

[5] **G. T. Craven**, T. Bartsch, and R. Hernandez
"Communication: Transition state trajectory stability determines barrier crossing rates in chemical reactions induced by time-dependent oscillating fields"
J. Chem. Phys. 141, 041106 (2014)

[4] **G. T. Craven**, A. V. Popov, and R. Hernandez
"Structure of a tractable stochastic mimic of soft particles"
Soft Matter 10, 5350 (2014)

[3] **G. T. Craven**, T. Bartsch, and R. Hernandez
"Persistence of transition state structure in chemical reactions driven by fields oscillating in time"
Phys. Rev. E 89(4), 040801(R) (2014)

[2] **G. T. Craven**, A. V. Popov, and R. Hernandez
"Stochastic dynamics of penetrable rods in one dimension: Occupied volume and spatial order"
J. Chem. Phys. 138, 244901 (2013)

[1] V. K. Dolmatov, **G. T. Craven**, E. Guler, and D. Keating
"Revivification of confinement resonances in the photoionization of A@C_{60} endohedral atoms far above thresholds"
Phys. Rev. A 80, 035401 (2009)

Proceedings

[2] V. K. Dolmatov, **G. T. Craven**, and D. Keating
"Confinement and electron correlation effects in photoionization of atoms in endohedral anions: Ne@C_{60}^{z-}"
J. Phys. Conf. Ser. 212, 012015 (2010)

[1] V. K. Dolmatov, **G. T. Craven**, E. Guler, and D. Keating
"Far above threshold confinement resonances in A@C_{60} atoms"
J. Phys. Conf. Ser. 194, 022025 (2009)

Technical Reports

[2] **G. T. Craven** and B. M. Wilson
"Generalized kinetic model for defect evolution in irradiated materials"
Los Alamos Technical Report LA-UR-23-25179 (2023)

[1] **G. T. Craven**
"Analytical solutions of the Arrhenius-Semenov problem for constant volume burn"
Los Alamos Technical Report LA-UR-21-31229 (2021)

Selected Presentations (out of ≈20 invited talks and ≈15 contributed talks)

[18] "Flow Field Analysis of Nonequilibrium Chemical Processes"
APS March Meeting, Minneapolis, MN (2024)

[17] "Molecular heat transport across an oscillating temperature gradient"
Discrete Simulation of Fluid Dynamics Conference, Albuquerque, NM (2023)

[16] "Electronic and phononic heat transport in nonequilibrium molecular systems"
Workshop on Chemical Dynamics in Complex Environments, Telluride, CO (2023)

[15] "Flow field analysis of nonequilibrium molecular reaction dynamics"
SIAM (Society for Industrial and Applied Mathematics) Conference on Dynamical Systems, Portland, OR (2023)

[14] "Nonequilibrium chemical dynamics: molecules, nanodevices, and materials"
Washington State University, Pullman, WA, (2023)

[13] "Electron hopping heat transport in molecules"
APS March Meeting, Las Vegas, NV (2023)

[12] "Machine learning approaches for thermodynamic and transport properties of fluids and materials"
Los Alamos - Arizona Days Conference, Los Alamos, NM (2021)

[11] "Upside/Downside statistical mechanics: What can economics tell us about thermodynamics?"
Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM (2021)

[10] "Electron transfer in thermally heterogeneous environments"
University of California, Los Angeles (UCLA), Los Angeles, CA (2020)

[9] "Machine learning approaches of structural and thermodynamic properties of fluids"
Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM (2020)

[8] "Upside/Downside statistical mechanics: What can economics tell us about thermodynamics?"
Physics and Chemistry of Materials Group meeting
Los Alamos National Laboratory (2019)

[7] "Electron transfer in thermally heterogeneous environments"
Workshop on Nonequilibrium Phenomena, Nonadiabatic Dynamics, and Spectroscopy, Telluride, CO (2019)

[6] "Electron transfer in thermally heterogeneous environments: A new paradigm for heat transport between molecules and at molecule-metal interfaces"
ACS National Meeting, Washington D.C. (2017)

[5] "Geometrical descriptors of time-dependent transition states"
Workshop on Nonequilibrium Statistical Physics, Telluride, CO (2016)

[4] "Geometrical descriptors of time-dependent transition states"
— Selected for the "Emerging Technologies in Computational Chemistry" Symposium —
ACS National Meeting, Philadelphia, PA (2016)

[3] "Multithermal currents in charge transfer reaction networks"
ACS National Meeting, Philadelphia, PA (2016)

[2] "Transition state theory for driven reactions"
Georgia Tech Chemistry Graduate Student Awards Symposium (2014)

[1] "Stochastic potentials for coarse-grained solvents"
Universidad Politéchnica de Madrid, Madrid, Spain (2013)

Service

- Independent Referee for: *J. Chem. Phys.*, *Nano Lett.*, *ACS Nano*, *J. Phys. Chem.*, *Nanoscale*, *Phys. Rev. Lett.*, *Phys. Rev. A*, *Phys. Rev. B*, *Phys. Rev. E*, *Phys. Rev. Research*, *PRX Quantum*, *PRX Energy*, *Communications Physics*, *Scientific Reports*, *Commun. Nonlinear Sci. Numer. Simul.*, *Science Advances*, *Ind. Eng. Chem. Res.*, *AIP* Publishing
- Reviewer for National Institute of Standards and Technology (NIST) Washington Editorial Review Board
- Theoretical Division Red Team (Proposal Review Panel), Los Alamos National Laboratory *2021 - current*
- LDRD AMQOS Exploratory Research Proposal Review Panel, Los Alamos National Laboratory *2024*
- Scientific Committee, International Conference on Advances in Mechanical Engineering and Mechanics *2024*
- Mentor, Los Alamos National Laboratory Computational Physics Summer School *2023*
- Organizer, CNLS Postdoc Seminar Series, Los Alamos National Laboratory *2020*
- Co-Organizer, Georgia Tech Research Symposium on Chemical Dynamics *2014*
- Georgia Tech PURA Reviewer (President's Undergraduate Research Awards) *2012, 2013*

Funding History

- Director's Initiative, Los Alamos National Laboratory, 2023-2026
  Project Title: Feedstocks, Optimization, and Requirements for Manufacturing
  Role: Co-Investigator
- Exploratory Research, Los Alamos National Laboratory, 2022-2025
  Project Title: Solving the Nonequilibrium Reaction Rate Problem Using Flow Fields
  Role: **PI**
- Exploratory Research, Los Alamos National Laboratory, 2022-2025
  Project Title: Physical, Geometric Machine Learning Models for Interacting 3D Objects
  Role: Co-Investigator
- Directed Research, Los Alamos National Laboratory, 2021-2024
  Project Title: Accelerating Nuclear Fuel Qualification through Integrated Multiscale and Multiphysics Models
  Role: **Co-PI**
- Director's Initiative, Los Alamos National Laboratory, 2020-2021
  Project Title: Data Driven Accelerated Fuel Qualification for Nuclear Fuels
  Role: Co-Investigator
- Director's Fellowship, Los Alamos National Laboratory, 2019-2021
  Project Title: *Ex Machina* Hamiltonians for Next-Generation Molecular Simulations
  Role: **PI**

Mentoring

Postdoctoral Associates

- Charlie Young (2023 - *current*)
  Los Alamos National Laboratory (T-1 Group and Center for Nonlinear Studies Fellow)
- Vidushi Sharma (2023 - *current*)
  Los Alamos National Laboratory (T-1 Group and Center for Nonlinear Studies Fellow)
- Emily Shinkle (2023 - *current*)
  Los Alamos National Laboratory (CCS-3 Group and T-1 Group)
- Renai Chen (2022 - *current*)
  Los Alamos National Laboratory (T-1 Group and Center for Nonlinear Studies Fellow)
- Sam Battey (2020 - 2022)
  Los Alamos National Laboratory (T-1 Group - now Scientist at LANL)

Mentoring Continued

Graduate Students

- Zachary Miller (2024)
  University of California, Berkeley
- Alex Guo (2024)
  University of Wisconsin - Madison
- Lucas Trojanowski (2023)
  University of Maryland
- Nicholas Dailey (2023)
  University of Illinois Urbana-Champaign
- Landon Johnson (2022 - 2024)
  North Dakota State University
- Renai Chen (2016 - 2019)
  University of Pennsylvania

High-School Students

- Manas Garg (2016)

Computing Grants

- Los Alamos National Laboratory Institutional Computing, 2024
  Project Title: Lagrangian Flow Analysis of Chemical Reaction Networks using GPU Architectures
  Role: **Co-PI**
  Amount: **2,000,000** GPU Hours
- Los Alamos National Laboratory Institutional Computing, 2024
  Project Title: Machine Learning Methods for Mechanistic Nuclear Fuel Model Development
  Role: **PI**
  Amount: **5,000,000** CPU Hours
- Los Alamos National Laboratory Institutional Computing, 2023-2025
  Project Title: Flow Field Analysis of Nonequilibrium Chemical Reactions
  Role: **PI**
  Amount: **7,300,000** CPU Hours
- Los Alamos National Laboratory Institutional Computing, 2022-2024
  Project Title: Machine Learning Methods for Mechanistic Models of Nuclear Fuels
  Role: **PI**
  Amount: **6,500,000** CPU Hours

Outreach

(1) I was a mentor at the 2023 Computational Physics Workshop at Los Alamos National Laboratory. I mentored two graduate students on a project focused on nonequilibrium chemical reaction dynamics.

(2) I have developed several interactive educational applets illustrating fundamental concepts in chemical reaction dynamics and dynamical systems theory: These applets have been used in various projects including artistic designs, books, and graphic design projects.

- Trajectories on the Müller-Brown Potential Energy Surface
- Rabinovich-Fabrikant Equations
- Phase Plane Trajectories of the Unforced Duffing Oscillator
- Chaotic Dynamics of a Magnetic Pendulum