Elizabeth J. Hartung

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EDUCATION

PhD Mathematics, Syracuse University, August 2012
- **Thesis:** *The Clar Structure of Fullerenes*, Syracuse University.
- **Advisor:** Jack E. Graver

MS Mathematics, Syracuse University, May 2008

BS Mathematics, Indiana University of Pennsylvania, May 2006

RESEARCH INTERESTS

My primary area of research is chemical graph theory, with special interests in fullerenes and benzenoids. Much of this work is on the Clar and Fries numbers of chemical graphs. My work has provided a theoretical understanding for empirical observations, such as in capped carbon nanotubes. I have also worked in combinatorial generation, pattern-avoiding permutations, computational geometry, and planar graphs.

AWARDS

Chemical Graphs on Steroids, Bilateral Research Grant, ARRS   2021

Grant Awarded by ARRS (Agency of Research of the Republic of Slovenia) to support research collaboration with Nino Bašić at the University of Primorska, Slovenia.

Faculty Incentive Award for Research, MCLA   2021

Course release awarded to support collaborative research in chemical graph theory.

Faculty Incentive Award for Sabbatical Research, MCLA   2018

Funding awarded to support in chemical graph theory.

40 Under Forty, Berkshire County   2017

Recognized as one of 40 individuals under 40 years old in the Berkshires for professional accomplishments and work in the community

Faculty Incentive Award for Research, MCLA   2015

Course release awarded for research in chemical graph theory.

Outstanding Teaching Assistant Award, Syracuse University   2011

The Outstanding TA Award is given to approximately the top 4 percent of all graduate student instructors campus wide.

PUBLICATIONS

(1) E. Downing, S. Einstein, E. Hartung, A. Williams, Catalan Squares and Staircases: Relayering and Repositioning Gray Codes, *Canadian Conference on Computational Geometry* (2023).

(2) Graver, J.E., Hartung, E.J., The Clar numbers of carbon nanotubes, *MATCH Commun. Math. Comput. Chem.* **87** (2022), 629-644.

(3) E.J. Hartung, H. Huang, T. Mutze, A. Williams, Combinatorial generation via permutation languages. I. Fundamentals, *Transactions of the American Mathematical Society*, **375** (2022), 2255-2291.

(4) Fowler, P.W., Myrvold, W., Vandenberg, R.L., Hartung, E.J., Graver, J.E., Clar and Fries structures for fullerenes. To appear in *The Art of Discrete and Applied Mathematics* (2022).

(5) Baes, A., Demaine, E.,D., Demaine, M.L., Hartung, E.J., Langerman, S., O'Rourke, J., Uehara, R., Uno, Y., Williams, A., Rolling Polyhedra on Tessellations, *FUN With Algorithms* (2022).

(6) Graver, J.E., Hartung, E.J., Williams, A. Resonance structures and aromaticity for capped carbon nanotubes, *Carbon*, **173** (2021), 1082-1092.

(7) Hartung, E.J., Huang, Mutze, T, Williams, Combinatorial Generation via Permutation Languages. *SODA (Symposium on Discrete Algorithms)*, (2020).

(8) Graver, J.E., Hartung, E.J., The Combinatorial Structure of Graphene. In: *Handbook of Graphene: Volume 2*, Tobias Stauber. Scrivener Publishing, pp. 73-94 (2019).

(9) J. Chapman, J. Foos, Hartung, E.J., A. Nelson, A. Williams. Pairwise Disagreements of Kekule, Clar, and Fries Numbers for Benzenoids: A Mathematical and Computational Investigation, *MATCH Commun. Math. Comput. Chem.* **80** (2018).

(10) Graver, J.E., Hartung, E.J., The Clar and Fries Structures of a Fullerene I, *Discrete Applied Mathematics* **216** (2016).

(11) Graver, J.E., Hartung, E.J., Internal Kekulé structures for Graphene and General Patches, *MATCH Commun. Math. Comput. Chem.*, **76** 3 (2016) pp. 693-705.

(12) Hartung, E.J., Clar Chains and a Countexample, *Journal of Mathematical Chemistry*, (2014) **52**, pp. 990-1006.

(13) Graver, J.E., Hartung, E.J., Kekuléan Benzenoids, *Journal of Mathematical Chemistry* (2014) **52**, pp. 977-989.

(14) Graver, J.E., Hartung, E.J., Self-dual Spherical Grids, *Electronic Journal of Combinatorics* (2014) **21**.

(15) Hartung, E.J., Fullerenes with complete Clar Structure, *Discrete Applied Mathematics* (2013) **161**, pp. 2952-2957.

(16) Graver, J.E., Hartung, E.J., Souid, A.Y., Clar and Fries Numbers for Benzenoids, *Journal of Mathematical Chemistry* (2013), **51**, pp. 1981-1989.

(17) Hartung, E.J. *The Clar Structure of Fullerenes*, Doctoral Thesis, Syracuse University, Syracuse, NY (2012).

TEACHING EXPERIENCE

Full Professor, Massachusetts College of Liberal Arts	2021-Present
Associate Professor, Massachusetts College of Liberal Arts	2016-2021
Assistant Professor, Massachusetts College of Liberal Arts	2011-2016

Courses Taught: Linear Algebra, Calculus I, II, and IV, Real Analysis, Calculus for High School Teachers, Graph Theory for Math Educators, Graph Theory I and II, Topology, Statistics and Data Analysis, Set Theory and Logic, Proof II, Intro to Statistics, Math for

Elementary Educators II and III, First Year Experience, Discrete Math, Abstract Algebra, Probability Theory, MTEL Prep Course, Fullerenes and Carbon Molecules, Topics in Chemical Graph Theory I and II, STEM Academy.

RELATED EXPERIENCE

Feigenbaum Fall Research Institute
Supervisor of undergraduate student in pattern-avoiding permutations.   2023

MCLA Summer Research Institute
Supervisor of undergraduate student in combinatorial generation. This collaboration resulted in a co-publication with two students.   2023

Virtual Workshops on Computational Geometry, participated in three week-long virtual workshops organized by Erik Demaine.   Spring 2020, 2021, 2022

Research visit TU Berlin Worked with Torsten Mutze and Aaron Williams at TU Berlin on Combinatorial Generation.   Summer, 2018

MCLA Summer Research Institute
Supervisor of undergraduate student in chemical graph theory   2018

Geometry of Redistricting Workshop
Participant in Tuft's workshop on the mathematics of redistricting and voting rights and a specialized Educator Track   2017

The Fullerene Project: Pilot Grant
MCLA leader in collaborative research project with Syracuse University. Mentored MCLA and Syracuse undergraduates and graduate students in chemical graph theory, particularly computing the Clar and Fries numbers for infinite classes of fullerenes. This work was supported by a pilot grant from Syracuse University. A paper with these results is in preparation.   Spring 2016

MCLA Summer Research Institute
Supervisor of two undergraduate students researching chemical graph theory   2014

CONFERENCE TALKS

35th Canadian Conference on Computational Geometry,   August 2023
Montreal, Canada
Catalan Squares and Staircases: Relayering and Repositioning Gray Codes

10th Slovenian Conference on Graph Theory,   June 2023
Kranjska Gora, Slovenia
Results on the Clar numbers of fullerenes

SIAM Conference on Discrete Mathematics,   June 2022
Carnegie Mellon University, Pittsburgh
Resonance Structures of Capped Carbon Nanotubes

Canadian Discrete and Algorithmic Mathematics Conference,   May 2021

Virtual Conference
Resonance Structures and Aromaticity in Capped Carbon Nanotubes

Coast Combinatorics Conference,   February 2019
University of Hawaii, Manoa
Aromaticity and Stability for Carbon Nanotubes

SIAM Conference on Discrete Mathematics,   June 2018
University of Colorado, Denver
The Fullerene Project

Ontario Combinatorics Workshop, Invited Speaker   June 2017
University of Guelph, Guelph, Canada
Fullerenes and Graphene Patches

Canadian Discrete and Algorithmic Mathematics Conference,   June 2017
Ryerson University, Toronto, Canada
Pairwise Incompatibility of Predictors of Stability for Graphene Patches

Meeting of the International Academy of Mathematical Chemistry & International Conference on Mathematical Chemistry, Invited Speaker   July 2016
Nankai University, Tianjin, China
Internal Kekulé structures for Graphene and General Patches (speaker)
Pairwise Incompatibility of the Kekule, Fries, and Clar Numbers for Benzenoids (co-author)
Session Chair

Computers in Scientific Discovery, Invited Keynote Speaker   July 2015
Virginia Commonwealth University, Richmond, VA
The Clar and Fries Numbers of Fullerenes and Benzenoids

8th Slovenian Conference on Graph Theory   June 2015
Kranjska Gora, Slovenia
The Clar and Fries Structures of a Fullerene
Session Chair

International Academy of Mathematical Chemistry   June 2015
Kranjska Gora, Slovenia
The Clar and Fries Structures of a Fullerene

Canadian Discrete and Algorithmic Mathematics Conference   June 2015
University of Saskatchewan, Saskatoon, Saskatchewan, CA
The Kekulé Count and Clar Number of Benzenoids

Society for Industrial and Applied Mathematics   June 2014
Minneapolis, MN
Kekuléan Benzenoids

Canadian Discrete and Algorithmic Mathematics Conference   June 2013
University of Newfoundland, Newfoundland, CA
The Clar Structure of a Fullerene

Society for Industrial and Applied Mathematics   June 2012
Dalhousie University, Halifax, Nova Scotia, CA

Self-Dual Plane Graphs with Maximum Degree 4

Canadian Discrete and Algorithmic Mathematics Conference   May 2011
University of Victoria, British Columbia, CA
Fullerene Parameters: A Colorful Approach

Computers in Scientific Discovery 5   July 2010
University of Sheffield, Sheffield, UK
Face Independence Numbers of Fullerenes

Discrete Math Day, Invited Speaker   May 2010
Worcester Polytechnic Institute, Worcester, MA
Fullerenes and Carbon Molecules

Canadian Discrete and Algorithmic Mathematics Conference   May 2009
University of Montreal, Montreal, CA
A Catalog of Self-Dual Plane Graphs with Maximum Degree 4

AMS Sectional Meeting   April 2009
Worcester Polytechnic Institute, Worcester, MA
A Catalog of Self-Dual Plane Graphs with Maximum Degree 4

PRESENTATIONS BY MENTORED STUDENTS

Women in Mathematics in New England, Smith College   September 2023
Emily Downing, "Cool-lex Order for Triangulations of Polygons"

MCLA Undergraduate Research Conference, MCLA   Spring 2023
Emily Downing, "Cool-lex Order for Triangulations of Polygons"

MCLA Undergraduate Research Conference, MCLA   Spring 2019
Paul Steven Davila and William Fines-Kested, "What Makes a Fullerene: The Quest for Kekule Numbers"

MCLA Undergraduate Research Conference, MCLA   Spring 2016
Selected students from Graph Theory II presented their research projects.
- Ian Angell and Satchel Lefebvre, "Finding the Clar and Fries Numbers for Infinite Classes of Graphs"
- Josh Colon, "Applied Electrical Circuit Analysis with Graph Theory"
- Allison Gaylock, "Vertex Coloring Game"
- Rebecca Godbout and Kayla Lavoice, "Using Graph Theory to Analyze Social Networks"

National Conference for Undergraduate Research, Washington State   Spring 2015
James Chapman and Andrew Nelson, "A Search for the Kekuleaness and Upper Bounds on the Clar and Fries Numbers of a Benzenoid."
Research supervised in independent studies Topics in Chemical Graph Theory I and II.

Statewide Undergraduate Research Conference, UMass Amherst   Spring 2015
James Chapman and Andrew Nelson,"A Search for the Kekuleaness and Upper Bounds on the Clar and Fries Numbers of a Benzenoid."
Research supervised in independent studies Topics in Chemical Graph Theory I and II.

Pokemon and Probability, MCLA Math Colloquium   Spring 2015
Heather Chiros presented research supervised in the courses "Discrete Mathematics" and "Graph Theory II"

MCLA Undergraduate Research Conference, MCLA   Spring 2015
James Chapman and Andrew Nelson, "Combinations of Graphs, Infinite Classes, and the Disproval of a Clar-Kekule Conjecture"

Statewide Undergraduate Research Conference, UMass Amherst   Spring 2014
James Chapman, "The Quest for Upper Bounds on Clar and Fries Numbers for Benzenoids"

MCLA Undergraduate Research Conference, MCLA   Spring 2014
Selected students from Graph Theory II presented their research projects.
- Ross Betti, "Constellations through Graph Theory"
- James Chapman, "The Quest for Upper Bounds on Clar and Fries Numbers for Benzenoids"
- Amory Galili, "Graph Maker"
- Patrick Munier, "The Human Brain and Mental Illness Examined through Graph Theory"

SERVICE

Department Chair   Fall 2022-Present
Served as Chair of the Math Department.

Discrete Mathematical Chemistry Journal, Editorial Board   Spring 2022-Present
Carried papers through the editing process, refereed papers and selected referees.

Data Science Minor Coordinator   Fall 2023-Summer 2024
Advised Minors, coordinated with faculty, shepherded changes to the Minor through governance.

Math Drop-in Center Coordinator,   Fall 2023-Summer 2024
Hired and trained peer tutors, created schedules, advertised the Drop-in Center, created review materials, maintained website, collected data.

Data Science Advisory Board, Member   Fall 2021-Present
Helped to create a new Data Science Minor at MCLA, which is in effect starting Fall 2022. Created course in new minor, working with curriculum for upper level courses in minor.

Committee on Tenure   2020-2022
Served as one of two faculty on the Committee on Tenure. Evaluated tenure applications, met with departments and candidates, wrote recommendations to the Vice President of Academic Affairs.

Peer Faculty Mentor   Fall 2021-Spring 2022
Served as the scholarship mentor for the Faculty Mentoring Network program through the Center for Teaching and Learning.

Minisymposium Organizer   May 2021
Co-organized a 15-speaker minisymposium in chemical graph theory for the virtual CanaDAM (Canadian Discrete and Algorithmic Mathematics) 2021 conference.

Lead Faculty Member for Math Drop-in Center   Fall 2017-Fall 2018

Wrote grant proposal to fund a new MCLA Math Drop-in Center. Hired students, provided training, advertised center, ran monthly meetings with peer tutors, met weekly with head tutor, collected data.

Quantitative Understanding Across the Curriculum, Member   Fall 2015-Present

Discussed and implemented strategies for improving quantitative understanding across disciplines, including starting the Math Drop-in Help Center

Peer Reviewer   Fall 2013-Present

Reviewed mathematical journal articles and grants for:
- *Discrete Mathematical Chemistry*
- *The Journal of Applied Mathematics*
- *Discrete Applied Mathematics*
- *Ars Mathematica Contemporaria*
- *Discussiones Mathematicae Graph Theory*
- *MATCH Commun. Math. Comput. Chem.*
- *Journal of Information Processing*
- NSF grant in chemical graph theory

Undergraduate Research Council, Member   Fall 2015-Present

Helped plan and organize the Undergraduate Research Conference, reviewed undergraduate proposals for funding.

STEM Pathways Program, Co-PI   Fall 2013-Spring 2019

Co-Principal Investigator on a successful NSF grant application for STEM Pathways program.

Math Society, Advisor   Fall 2013-Spring 2018

Advise this student group; take students on field trips and to conferences; help organize student events.

Community-Based Learning Group, Faculty Co-coordinator Spring 2013-Spring 2020

Encourage community-based learning in MCLA courses, meet with faculty members to discuss ideas for courses and logistics, serve as a liaison between faculty and community partners.

Math Alignment Group, MCLA Representative   Spring 2012-Spring 2019

Connect with local teachers, principals, and math coaches in area to discuss common interests.
- Regular math alignment meetings with Berkshire county teachers and professors.
- Co-facilitated *Diving Deeper*, a workshop for principals, math teachers, and math coaches in implementing new common core standards.
- Participated in Train-the-Trainer Workshop

Monument Mountain Regional High School Self-Study, Community Partner Spring 2016

Met with faculty, administrators, and students at Monument Mountain Regional to assess and report back to the administration and mathematics department. This self-study was used as an alternative assessment to NEASC.

Developmental Math Advisory Board, MCLA Representative   Spring 2014-Fall 2016

Work with the department of higher education and CSSE to determine policies for developmental math courses and placement.

MCLA Alternative Spring Break

Group leader for student service learning trip to Belize.   March 2014

Brought 18 students to Belize, where we engaged in cultural exchange, brought school supplies, built sidewalks and did maintenance at an elementary school.