

## **Mark L. Elert**

---

Chemistry Department  
U. S. Naval Academy  
572 Holloway Rd.  
Annapolis, MD 21402-5026

2027 Huntwood Dr.  
Gambrills, MD 21054  
410-721-0322 (home)

410-293-6636 (office)  
410-293-2218 (FAX)  
elert@usna.edu

### **Education**

1968—1972 Michigan State University  
B.S. in chemical physics, 1972

1972—1976 University of California at Berkeley  
Ph.D. in physical chemistry, 1977

NSF Graduate Fellow (1972-1975)

Dissertation Topic:  
A Case Study of Predissociation Dynamics in Small Polyatomic Molecules: Formaldehyde

Advisor: W. M. Gelbart

### **Professional Employment**

University of California, Los Angeles, CA  
Department of Chemistry

1977—1979 Adjunct Assistant Professor

U. S. Naval Academy, Annapolis, MD  
Chemistry Department

1979—1983 Assistant Professor  
1983—1988 Associate Professor  
1988— Professor  
1988—1990 Associate Chairman  
1990—1994 Chairman  
2006—2010 Chairman

## **Mark L. Elert**

---

### **Professional Society Involvement**

#### **American Physical Society**

Technical Program Committee, APS Conference on Shock Compression of Condensed Matter, Williamsburg, VA, June 1991.

Nominating Committee, APS Topical Group on Shock Compression of Condensed Matter, 1992-1993.

Co-chair, APS Conference on Shock Compression of Condensed Matter, 2005.

Selection Committee for American Physical Society "Shock Compression Research Award," 2005-2007.

### **Honors and Awards**

Alumni Distinguished Scholar, Michigan State University, 1968–1972

Phi Beta Kappa

National Science Foundation Graduate Fellow, 1972–1975

Chemistry Department Nominee, USNA Faculty Award for Excellence in Teaching, 1987

Chemistry Department Nominee, USNA Faculty Award for Excellence in Research, 1988

Winner, USNA Faculty Award for Excellence in Research, 1992

Navy Meritorious Civilian Service Medal, 1992

Chemistry Department Nominee, USNA Service Excellence Award, 1998 and 1999

Navy Meritorious Civilian Service Medal, 1999

### **Recent Institutional Service**

Chair, Faculty Senate Curriculum Committee, 2010-

The FSCC has overall responsibility for recommending changes to the Naval Academy curriculum. Subcommittees of the FSCC handle curriculum change requests for the core curriculum and the academic divisions; these subcommittees report to the FSCC.

Member, Navy Selection Board for the new Junior Permanent Military Professor program, 2010

Traveled to Navy Personnel Command in Millington Tennessee to select officers for permanent duty as instructors at the Naval Academy. The Selection Board was chaired by the Superintendent.

Member, Permanent Military Professor Continuation Board, 2010

Considered requests for Permanent Military Professors to continue to serve beyond their statutory retirement date.

## **Mark L. Elert**

---

### **Recent Institutional Service (cont'd.)**

Chair, Search Committee for Naval Academy Preparatory School Academic Dean, 2010

Chair, Chemistry Department, 1990–1994 and 2006–2010

Manage large academic department with approximately 40 faculty members, eight technicians, and more than 50,000 square feet of laboratory and classroom space. The department teaches a large general chemistry core course for all 1200 plebes each year, and an ACS-accredited majors program with about 35 students per year.

Member, Committee on Technical Support, 2005–2006

This committee was formed to examine the current status, needs, and requirements for technical support at the Naval Academy, primarily in the Divisions of Engineering & Weapons and Mathematics & Science.

Co-chair, Naval Academy Research Council (NARC), 2005–2006

Select recipients of internal Naval Academy research grants.

Member, Faculty Senate, 1995–1999, 2005–2006, 2010–

The Faculty Senate consists of approximately 35 members elected from the full faculty of 650. It acts as an advisory body to the administration on a wide range of faculty-related issues.

Member of the Faculty Senate Executive Committee, 1998–1999, 2005–2006

The Executive Committee is composed of the Senate's three officers and four other members elected by the Senate. The Executive Committee sets the agenda for Senate meetings, acts for the Senate on matters requiring attention between regular Senate meetings, and appoints Senate committee chairs and members.

Member, Naval Academy Promotion and Tenure Committee, 1998–2003

Committee members visit classes of potential candidates for promotion during the fall semester. During a six-week period from late January through early March, the committee meets for several hours almost daily to review promotion packages, interview department chairs, and deliberate about promotion recommendations. The committee then meets with the Academic Dean to review its findings and present its recommendations.

Chair, Academic Affairs Committee, Faculty Senate, 1995–1998

The Academic Affairs Committee serves as the primary agent of the Senate in dealing with issues related to the academic concerns of the institution, most especially teaching and scholarship.

Member of the Core Team, “Curriculum 21” Review, 1997–1998

The Superintendent of the Naval Academy established the Curriculum 21 group to “monitor demands on midshipmen, to optimize the balance between academic and professional development, and determine the proper balance between Humanities/Social Sciences and Math, Science, and Engineering in the curriculum.” The committee met with fleet commanders and other senior Navy and Marine Corps leaders to determine the skills and attributes needed for future officers into the twenty-first century. After a five-month intensive study of the core curriculum and professional training at the Naval Academy, the group made several substantive recommendations to the Superintendent for improvements in both areas.

## **Mark L. Elert**

---

### **Recent Institutional Service (cont'd.)**

Member, Academic Dean Search Committee, 1997

The Committee was responsible for conducting a nationwide search for a new Chief Academic Officer for the Naval Academy. The Committee examined more than 170 applications, interviewed 16 semifinalists, invited 5 finalists to the campus for two-day visits, and conducted site visits at the current institutions of three candidates. The search was completed successfully in July 1997.

Senior Academic Adviser, Chemistry Department, 1994–2005

The Senior Academic Adviser is responsible for overseeing the advising program for the department. Responsibilities include handling scheduling and registration problems for chemistry majors, assisting students who wish to change majors or participate in exchange programs with other service academies, and ensuring that students meet graduation requirements.

## **Mark L. Elert**

---

### **Publications**

1. 'Decays, Recurrences, and Large Molecule Behavior in the Theory of Radiationless Transitions', W. M. Gelbart, D. F. Heller, and **M. L. Elert**, *Chem. Phys.* **7**, 116–122 (1975).
2. 'Local Mode Structure of the Water Molecule', **M. L. Elert**, P. R. Stannard, and W. M. Gelbart, *J. Chem. Phys.* **67**, 5395–5396 (1977).
3. 'Photodissociation Dynamics of Small Polyatomics: Isolated Molecule Behavior and Collision-Induced Effects', D. F. Heller, **M. L. Elert**, and W. M. Gelbart, *J. Chem. Phys.* **69**, 4061–4067 (1978).
4. 'Some Symmetry Aspects of the Local-Mode Description of Vibrational Structure', W. M. Gelbart, P. R. Stannard, and **M. L. Elert**, *Int. J. Quantum Chem.* **14**, 703–708 (1978).
5. 'Photodissociation of the Formaldehyde Molecule: Does It or Doesn't It?', W. M. Gelbart, **M. L. Elert**, and D. F. Heller, *Chemical Reviews* **80**, 403–416 (1980).
6. 'On the Overtone-Combination Spectra of XY<sub>2</sub> Molecules', P. R. Stannard, **M. L. Elert** and W. M. Gelbart, *J. Chem. Phys.* **74**, 6050–6062 (1981).
7. 'Component Vapor Pressures as a Function of Initial Quantity of Solution', E. Koubek and **M. L. Elert**, *J. Chem. Ed.* **59**, 357–359 (1982).
8. 'The Effects of Off-Diagonal Disorder on Soliton- and Polaron-like States in *trans*-Polyacetylene', C. T. White, **M. L. Elert**, and J. W. Mintmire, *J. Phys. Paris, Colloq.* **44**, C3/481–484 (1983).
9. 'Cross-links in Polyacetylene', C. T. White, P. Brant, and **M. L. Elert**, *J. Phys. Paris, Colloq.* **44**, C3/443–446 (1983).
10. 'Tight-Binding Studies for Electroactive Organic Polymers', **M. L. Elert**, J. W. Mintmire, and C. T. White, *J. Phys. Paris, Colloq.* **44**, C3/451–454 (1983).
11. 'Helical versus Planar *cis*-Polyacetylene', **M. L. Elert** and C. T. White, *Phys Rev. B (Rapid Comm.)* **28**, 7387–7389 (1983).
12. 'Conformation and Electronic Properties of Helical *cis*-Polyacetylene', **M. L. Elert**, C. T. White, and J. W. Mintmire, *Mol. Cryst. Liq. Cryst.* **125**, 329–335 (1985).
13. 'Local-Density Functional Approach to Chain Polymers', J. W. Mintmire, C. T. White, and **M. L. Elert**; *Mol. Cryst. Liq. Cryst.* **125**, 337–343 (1985).
14. 'Calculation of Madelung Constants in the First Year Chemistry Course', **M. L. Elert** and E. Koubek, *J. Chem. Ed.* **63**, 840–841 (1986).
15. 'Heteroatom Effects in Heterocyclic Ring Chain Polymers', J. W. Mintmire, C. T. White, and **M. L. Elert**, *Synth. Metals* **16**, 235–243 (1986).
16. 'Lattice Parameters and Packing Energies for Helical Polyacetylene', **M. L. Elert** and C. T. White, *Macromolecules* **20**, 1411–1414 (1987).
17. 'Conformation and Electronic Structure of Heterocyclic Ring Chain Polymers', J. W. Mintmire, C. T. White, and **M. L. Elert**, *Synth. Metals* **25**, 109–119 (1988).

## **Mark L. Elert**

---

### Publications (cont'd.)

18. 'One-dimensional Molecular-dynamics Simulation of the Detonation of Nitric Oxide', **M. L. Elert**, D. M. Deaven, D. W. Brenner, and C. T. White, *Phys. Rev. B (Rapid Comm.)* **39**, 1453–1456 (1989).
19. 'Chemical Model for Intrinsic Detonation Velocities', D. W. Brenner, C. T. White, **M. L. Elert**, and F. E. Walker, *Int. J. Quantum Chem., Quantum Chemistry Symposium* **23**, 333–337 (1989).
20. 'Incorporation of Reactive Dynamics in Simulations of Chemically-Sustained Shock Waves', D. W. Brenner, **M. L. Elert**, and C. T. White, Shock Compression of Condensed Matter – 1989, S. C. Schmidt, J. N. Johnson, L. W. Davison, eds., Elsevier Science Publishers B.V., 263–266 (1990).
21. 'Some One-Dimensional Molecular Dynamics Simulations of Detonation', **M. L. Elert**, D. W. Brenner, and C. T. White, Shock Compression of Condensed Matter – 1989, S. C. Schmidt, J. N. Johnson, L. W. Davison, eds., Elsevier Science Publishers B.V., 275–278 (1990).
22. 'Molecular Dynamics Simulations of Shock-Induced Chemistry: Application to Chemically Sustained Shock Waves', C. T. White, D. H. Robertson, **M. L. Elert**, and D. W. Brenner, Microscopic Simulations of Complex Hydrodynamic Phenomena, M. Mareschal and B. L. Holian, eds., Plenum Press, 111–123 (1992).
23. 'Description à l'échelle moléculaire des ondes de choc soutenues chimiquement', ('Molecular Description of Chemically Sustained Shock Waves'), C. T. White, D. H. Robertson, J. W. Mintmire, D. W. Brenner, and **M. L. Elert**, *Revue Scientifique et Technique de la Défense* **16**, 157–160 (1992).
24. 'Simulations of Chemically-Sustained Shock Fronts in a Model Energetic Material', D. W. Brenner, **M. L. Elert**, and C. T. White, Shock Compression of Condensed Matter – 1991, S. C. Schmidt, R. D. Dick, J. W. Forbes, D. G. Tasker, eds., Elsevier Science Publishers B.V., 123–126 (1992).
25. 'Dissociative Phase Transitions, Split Shock Waves, Rarefaction Shocks, and Detonations', C. T. White, D. H. Robertson, **M. L. Elert**, J. W. Mintmire, and D. W. Brenner, *Mat. Res. Soc. Symp. Proc.* **296**, 123–128 (1993).
26. 'Detonations at Nanometer Resolution Using Molecular Dynamics', D. W. Brenner, D. H. Robertson, **M. L. Elert**, and C. T. White, *Phys. Rev. Letters* **70**, 2174–2177 (1993).
27. 'Molecular Description of Chemically Sustained Shock Waves: From Initiation to Continuum Behavior in a Hundred Picoseconds', C. T. White, D. H. Robertson, J. W. Mintmire, D. W. Brenner, and **M. L. Elert**, Proceedings of TNO-RML/ONR Workshop on Desensitization of Explosives and Propellants, (1993).
28. 'Molecular Dynamics of Void Collapse Mechanisms in Shocked Media', J. W. Mintmire, D. H. Robertson, **M. L. Elert**, D. W. Brenner, and C. T. White, High-Pressure Science and Technology – 1993, S. C. Schmidt, J. W. Shaner, G. A. Samara, M. Ross, eds., AIP Press, New York, 969–972 (1994).
29. 'Effects of Intense Disturbances on the Model Shock Front Supported by Chemical Reactions', **M. L. Elert**, D. H. Robertson, and C. T. White, *Khimicheskaya Fizika* **14**, 41–46 (1995).
30. 'Molecular Dynamics Study of Reaction Zone Properties in Chemically Sustained Shock Waves', **M. L. Elert**, D. H. Robertson, J. J. C. Barrett, and C. T. White, Shock Compression of Condensed Matter – 1995, S. C. Schmidt and W. C. Tao, eds., AIP Press, New York, 183–186 (1996).
31. 'Molecular Dynamics Study of Chemistry from Strong Shock Waves Interacting with Voids', C. T. White, J. J. C. Barrett, J. W. Mintmire, **M. L. Elert**, and D. H. Robertson, Shock Compression of Condensed Matter – 1995, S. C. Schmidt and W. C. Tao, eds., AIP Press, New York, 187–190 (1996).

## **Mark L. Elert**

---

### Publications (cont'd.)

32. 'Effects of Nanoscale Voids on the Sensitivity of Model Energetic Materials', C. T. White, J. J. C. Barrett, J. W. Mintmire, **M. L. Elert**, and D. H. Robertson, *Mat. Res. Soc. Symp. Proc.* **418**, 277–280 (1996).
33. 'Molecular Dynamics Study of the Effect of Varying Exothermicity on the Properties of Condensed-Phase Detonation', **M. L. Elert**, D. H. Robertson, and C. T. White, *Mat. Res. Soc. Symp. Proc.* **418**, 309–312 (1996).
34. 'A Demonstration of Crystal-Field Effects in Octahedral Complexes', Edward Koubek and **M. L. Elert**, *J. Chem. Ed.* **73**, 947 (1996).
35. 'Investigation of Detonation Properties by Molecular Dynamics Simulations', **M. L. Elert**, J. J. C. Barrett, and C. T. White, (*Russian*) *Chem. Phys. Reports* **17**, 185–190 (1998).
36. 'Molecular Dynamics Investigation of the Effects of Variation in Energy Release on Detonation Initiation', **M. L. Elert**, J. J. C. Barrett, D. H. Robertson, and C. T. White, *Shock Compression of Condensed Matter – 1997*, S. C. Schmidt, D. P. Dandekar, and J. W. Forbes, eds., AIP Press, New York, 293–296 (1998).
37. 'Detonation Hugoniot for Ozone from Molecular Dynamics Simulation', J. J. C. Barrett, D. H. Robertson, **M. L. Elert**, and C. T. White, *Shock Compression of Condensed Matter – 1997*, S. C. Schmidt, D. P. Dandekar, and J. W. Forbes, eds., AIP Press, New York, 329–331 (1998).
38. 'Self-Similar Behavior from Molecular Dynamics Simulations of Detonations', D. H. Robertson, J. J. C. Barrett, **M. L. Elert**, and C. T. White, *Shock Compression of Condensed Matter – 1997*, S. C. Schmidt, D. P. Dandekar, and J. W. Forbes, eds., AIP Press, New York, 297–300 (1998).
39. 'Molecular Dynamics Simulation of Shock-Induced Chemistry in Acetylene', **M. L. Elert**, D. R. Swanson, and C. T. White, *Shock Compression of Condensed Matter – 1999*, M. D. Furnish, L. C. Chhabildas, and R. S. Hixson, eds., AIP Press, New York, 283–286 (2000).
40. 'Critical Widths in Molecular Dynamics Simulations of Detonations', C. T. White, D. H. Robertson, D. R. Swanson, and **M. L. Elert**, *Shock Compression of Condensed Matter – 1999*, M. D. Furnish, L. C. Chhabildas, and R. S. Hixson, eds., AIP Press, New York, 377–380 (2000).
41. 'Detonation Hugoniots Produced by Piston-Driven Simulations', D. R. Swanson, **M. L. Elert**, and C. T. White, *Shock Compression of Condensed Matter – 1999*, M. D. Furnish, L. C. Chhabildas, and R. S. Hixson, eds., AIP Press, New York, 385–388 (2000).
42. 'Molecular Dynamics Modeling of Impact-Induced Shock Waves in Hydrocarbons', **M. L. Elert**, Sergey Zybin, and C. T. White, *Shock Compression of Condensed Matter – 2001*, M. D. Furnish, N. N. Thadhani, and Y. Horie., eds., AIP Press, New York, 1406–1409 (2002).
43. 'Atomistic Modeling of Orientation Dependence of Shock Wave Properties in Diamond', Sergey Zybin, **M. L. Elert**, J. A. Harrison, and C. T. White, *Shock Compression of Condensed Matter – 2001*, M. D. Furnish, N. N. Thadhani, and Y. Horie, eds., AIP Press, New York, 355–358 (2002).
44. 'Orientation Dependence of Shock-Induced Chemistry in Diamond', Sergey Zybin, **M. L. Elert**, and C. T. White, *Phys. Rev. B (Rapid Comm.)* **66**, 220102-1(R) – 220102-4(R) (2002).
45. 'Molecular Dynamics Study of Shock-Induced Chemistry in Small Condensed-Phase Hydrocarbons', **M. L. Elert**, S. V. Zybin, and C. T. White, *J. Chem. Phys.* **118**, 9795–9801 (2003).

## **Mark L. Elert**

---

### **Publications (cont'd.)**

46. ‘Molecular Dynamics Study of Shock-Induced Chemistry in Anthracene’, M. L. Elert, S. V. Zybin, and C. T. White, Shock Compression of Condensed Matter – 2003, M. D. Furnish, Y. M. Gupta, and J. W. Forbes, eds., AIP Press, New York, 323–326 (2004).
47. ‘Molecular Dynamics Study of Non-Reacting Shock Waves in Anthracene’, S. V. Zybin, M. L. Elert, and C. T. White, Shock Compression of Condensed Matter – 2003, M. D. Furnish, Y. M. Gupta, and J. W. Forbes, eds., AIP Press, New York, 306–309 (2004).
48. ‘Molecular Dynamics Studies of Orientation Dependence of Shock Structure in Solids’, S. V. Zybin, V. V. Zhakhovskii, M. L. Elert, and C. T. White, Shock Compression of Condensed Matter – 2003, M. D. Furnish, Y. M. Gupta, and J. W. Forbes, eds., AIP Press, New York, 310–313 (2004).
49. ‘Nanoscale Modeling of Shock-Induced Deformation of Diamond’, S. V. Zybin, I. I. Oleynik, M. L. Elert, and C. T. White, *Mat. Res. Soc. Symp.* **800**, 299–304 (2004).
50. ‘Nanoscale View of Shock-Wave Splitting in Diamond’, S. V. Zybin, M. L. Elert, and C. T. White, *Metallurgical and Materials Transactions A* **35**, 2647–2650 (2004).
51. ‘Shock-Induced Chemistry in Hydrocarbon Molecular Solids’, M. L. Elert, S. V. Zybin, and C. T. White, chapter 12 in ‘Chemistry at Extreme Conditions’, M. R. Manaa, ed., Elsevier Press 351–368 (2005).
52. ‘Reactive Molecular Dynamics Simulations of Shock-Induced Chemistry in Hydrocarbons’, M. L. Elert, S. V. Zybin, and C. T. White, Lecture Series on Computer and Computational Sciences, vol. 4, T. Simos and G. Maroulis, eds., Bell Academic Publishers, The Netherlands, 1134–1137 (2005).
53. ‘Extreme Chemistry at the Nanoscale in Detonation Simulations’, C. T. White, D. R. Swanson, and M. L. Elert, Lecture Series on Computer and Computational Sciences, vol. 4, T. Simos and G. Maroulis, eds., Bell Academic Publishers, The Netherlands, 1130–1133 (2005).
54. ‘Quantum Dynamics of Energy Transfer under Shock Conditions’, R. C. Mowrey, M. L. Elert, and C. T. White, Shock Compression of Condensed Matter – 2005, M. D. Furnish, M. L. Elert, T. P. Russell, and C. T. White, eds., AIP Press, New York, 409–412 (2006).
55. ‘Shear Stresses in Shock-Compressed Covalent Solids’, I. I. Oleynik, S. V. Zybin, M. L. Elert, and C. T. White, Shock Compression of Condensed Matter – 2005, M. D. Furnish, M. L. Elert, T. P. Russell, and C. T. White, eds., AIP Press, New York, 417–420 (2006).
56. ‘Nanoscale Molecular Dynamics Simulation of Shock Compression of Silicon’, I. I. Oleynik, S. V. Zybin, M. L. Elert, and C. T. White, Shock Compression of Condensed Matter – 2005, M. D. Furnish, M. L. Elert, T. P. Russell, and C. T. White, eds., AIP Press, New York, 413–416 (2006).
57. ‘Molecular Dynamics Simulations of an Anomalous Response of Diamond to Shock Compression’, K. McLaughlin, I. I. Oleynik, S. V. Zybin, M. L. Elert, and C. T. White, Shock Compression of Condensed Matter – 2007, M. L. Elert, M. D. Furnish, R. Chau, N. C. Holmes, and J. Nguyen, eds., AIP Press, New York (2007).
58. ‘Shear Stresses in Shock-Compressed Diamond from Density Functional Theory’, I. I. Oleynik, A. C. Landerville, S. V. Zybin, M. L. Elert, and C. T. White, *Phys. Rev. B (Rapid Comm.)* **78**, 180101-1(R) – 180101-4(R) (2008).

## **Mark L. Elert**

---

### **Proceedings Edited**

1. "Shock Compression of Condensed Matter – 2005," Proceedings of the Conference of the American Physical Society Topical Group on Shock Compression of Condensed Matter, held in Baltimore, Maryland July 31 – August 5, 2005; M. D. Furnish, M. L. Elert, T. P. Russell, and C. T. White, eds., AIP Press, New York, 2006; AIP Conference Proceedings #845; ISBN 0-7354-0341-1.
2. "Shock Compression of Condensed Matter – 2007," Proceedings of the Conference of the American Physical Society Topical Group on Shock Compression of Condensed Matter, held in Waikoloa, Hawai'i, June 24 – June 29, 2007; M. L. Elert, M. D. Furnish, R. Chau, N. C. Holmes, J. Nguyen, eds., AIP Press, New York, 2007; AIP Conference Proceedings #955; ISBN 978-0-7354-0469-4.
3. "Shock Compression of Condensed Matter – 2009," Proceedings of the Conference of the American Physical Society Topical Group on Shock Compression of Condensed Matter, held in Nashville, Tennessee, June 28 – July 3, 2009; M. L. Elert, W. T. Buttler, M. D. Furnish, W. W. Anderson, and W. G. Proud, eds., AIP Press, New York, 2009; AIP Conference Proceedings #1195; ISBN 978-0-7354-0732-9.

### **Papers presented**

1. 'Intrinsic Defects in *trans*-Polyacetylene', **M. L. Elert**, Middle Atlantic Regional Meeting of the American Chemical Society, Washington, D.C., January 7, 1981.
2. 'Effects of Intrinsic Defects on the Electronic Structure of *trans*-Polyacetylene', **M. L. Elert**, American Conference on Theoretical Chemistry, Boulder, CO, June 23, 1981.
3. 'Effects of Disorder on Pople-Walmsley Defects in *trans*-Polyacetylene', C. T. White, **M. L. Elert**, and J. W. Mintmire, APS National meeting, Dallas, TX, March 11, 1982. [Bull. Amer. Phys. Soc. **27**, 375 (1982)]
4. 'Effects of Disorder on *trans*-Polyacetylene', C. T. White and **M. L. Elert**, 183rd American Chemical Society National Meeting, Las Vegas, Nevada, March 31, 1982. [Polymer Preprints **23**, 111 (1982)]
5. 'Tight-Binding Studies on Polyacetylene', **M. L. Elert** and C. T. White, 183rd American Chemical Society National Meeting, Las Vegas, Nevada, March 31, 1982. [Polymer Preprints **23**, 114 (1982)]
6. 'Tight-Binding Studies of Electroactive Organic Polymers', **M. L. Elert**, J. W. Mintmire, and C. T. White, International Conference on the Physics and Chemistry of Conducting Polymers (ICPCCP), Bourg-St.-Maurice, France, December 13, 1982.
7. 'The Effects of Off-Diagonal Disorder on Soliton- and Polaron-like States in *trans*-Polyacetylene', C. T. White, **M. L. Elert**, and J. W. Mintmire, International Conference on the Physics and Chemistry of Conducting Polymers (ICPCCP), Bourg-St.-Maurice, France, December 13, 1982.
8. 'Cross-links and Unpaired Spins in Polyacetylene', C. T. White, P. Brant, and **M. L. Elert**, International Conference on the Physics and Chemistry of Conducting Polymers (ICPCCP), Bourg-St.-Maurice, France, December 13, 1982.
9. 'Tetrahedral Crosslinks in Polyacetylene', C. T. White and **M. L. Elert**, APS National Meeting, Los Angeles, CA, March 21-25, 1983.
10. 'The Geometry of *cis*-Polyacetylene: A Quantum-Mechanical Study', **M. L. Elert** and C. T. White, APS National Meeting, Detroit, MI, March 26-30, 1984.

## **Mark L. Elert**

---

### **Papers presented (cont'd.)**

11. 'Helical *cis*-Polyacetylene: Geometry and Electronic Structure', **M. L. Elert** and C. T. White, Fifth American Conference on Theoretical Chemistry, Jackson, Wyoming, June 15-20, 1984.
12. 'Conformation and Electronic Properties of Helical *cis*-Polyacetylene', **M. L. Elert** and C. T. White, International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 16-21, 1984.
13. 'Electronic Structure Calculations for Heterocyclic Ring Chain Polymers', J. W. Mintmire, C. T. White, and **M. L. Elert**, APS National Meeting, Baltimore, MD, March 27, 1985 [Bull. Am. Phys. Soc. **30**, 471 (1985)].
14. 'Band Structure and Crystal Packing Calculations for Helical Polyacetylene', **M. L. Elert**, C. T. White, and J. W. Mintmire, APS National Meeting, Baltimore, MD, March 28, 1985 [Bull. Am. Phys. Soc. **30**, 566 (1985)].
15. 'First-Principles Results for the Geometry of *cis*-Polyacetylene', C. T. White, J. W. Mintmire, and **M. L. Elert**, APS National Meeting, New Orleans, LA, March 22, 1988 [Bull. Am. Phys. Soc. **33**, 457 (1988)].
16. 'Molecular Dynamics Simulation of the Detonation of Solid Nitric Oxide', **M. L. Elert** and D. M. Deaven, APS National Meeting, New Orleans, LA, March 22, 1988 [Bull. Am. Phys. Soc. **33**, ??? (1988)].
17. 'Simulations of Reactive Collisions in a Molecular Solid', D. W. Brenner, C. T. White, and **M. L. Elert**, APS National Meeting, St. Louis, MO, March 20-24, 1989 [Bull. Am. Phys. Soc. **34**, 608 (1989)].
18. 'Molecular Dynamics Simulations of Shock Waves in Model Energetic Materials', C. T. White, D. W. Brenner, **M. L. Elert**, and F. E. Walker, Sanibel Symposia, St. Augustine, Florida, April 1-8, 1989.
19. 'Simulation of a Chemically-Sustained Shock Wave in a Molecular Solid', D. W. Brenner, C. T. White, and **M. L. Elert**, Conference on the Dynamics of Molecular Collisions, Asilomar, CA, July 16-21, 1989.
20. 'Some One-Dimensional Molecular Dynamics Simulations of Detonation', **M. L. Elert**, D. W. Brenner, and C. T. White, APS Topical Conference on Shock Compression of Condensed Matter, Albuquerque, NM, August 14-17, 1989 [Bull. Am. Phys. Soc. **34**, 1722 (1989)].
21. 'Reaction Dynamics of a Chemically Sustained Shock Wave', D. W. Brenner, C. T. White, and **M. L. Elert**, APS Topical Conference on Shock Compression of Condensed Matter, Albuquerque, NM, August 14-17, 1989 [Bull. Am. Phys. Soc. **34**, 1722 (1989)].
22. 'Molecular Dynamics Simulations of the Onset of Detonation', **M. L. Elert**, D. W. Brenner, and C. T. White, International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 17-22, 1989.
23. 'Molecular-Dynamics Simulations of Shock-Induced Chemistry in Model Molecular Solids', C. T. White, D. W. Brenner, and **M. L. Elert**, APS National Meeting, Anaheim, CA, March 12-16, 1990 [Bull. Am. Phys. Soc. **35**, 698 (1990)].
24. 'Molecular-Dynamics Simulations of the Detonation of Nitric Oxide', **M. L. Elert**, D. W. Brenner, and C. T. White, APS National Meeting, Anaheim, CA, March 12-16, 1990 [Bull. Am. Phys. Soc. **35**, 698 (1990)].
25. 'Atomistic Simulations of Carbon in Shock Waves', D. W. Brenner, C. T. White, and **M. L. Elert**, APS National Meeting, Anaheim, CA, March 12-16, 1990 [Bull. Am. Phys. Soc. **35**, 699 (1990)].
26. 'Simulations of Reactive Collisions in Detonating Solids', **M. L. Elert**, D. W. Brenner, D. H. Robertson, and C. T. White, ONR Workshop on Rapid Crystalline Decomposition, Annapolis, MD, December 15, 1990.

## **Mark L. Elert**

---

### **Papers presented (cont'd.)**

27. 'Simulations of Condensed Phase Detonations', DRET/ONR Workshop on Understanding Detonations at the Molecular Level, Paris, France, June 7, 1991.
28. 'Simulations of Chemically-Sustained Shock Waves in Energetic Materials', D. H. Robertson, D. W. Brenner, **M. L. Elert**, and C. T. White, American Physical Society Conference on Shock Compression of Condensed Matter, Williamsburg, VA, June 17-20, 1991 [Bull. Am. Phys. Soc.; 36, 1829 (1991)].
29. 'Molecular Dynamics Simulations of Shock Induced Chemistry: Application to Chemically Sustained Shock Waves', C. T. White, D. H. Robertson, **M. L. Elert**, and D. W. Brenner, NATO Advanced Study Institute, Alghero, Italy, July 15-26, 1991.
30. 'Molecular Description of Chemically-sustained Shock Waves: From Initiation to Continuum Behavior in a Hundred Picoseconds', C. T. White, D. H. Robertson, J. W. Mintmire, D. W. Brenner, and **M. L. Elert**, ONR Workshop on Desensitization of Explosives and Propellants, Delft, Netherlands, November 13, 1991.
31. 'Chemical Dynamics Simulations as a Probe of the Initiation and Propagation of Condensed Phase Detonations', C. T. White, D. H. Robertson, **M. L. Elert**, and D. W. Brenner, ONR/LANL Workshop on the Fundamental Physics and Chemistry of Combustion, Initiation, and Detonation of Energetic Materials, Los Alamos, New Mexico, March 4, 1992.
32. 'Shock Waves and Polymorphic Phase Transitions in Energetic Materials', D. H. Robertson, D. W. Brenner, **M. L. Elert**, and C. T. White, ONR/LANL Workshop on the Fundamental Physics and Chemistry of Combustion, Initiation, and Detonation of Energetic Materials, Los Alamos, New Mexico, March 4, 1992.
33. 'Molecular Dynamics Simulations of Detonations: From Atomic Scale to Continuum Behavior in under a Hundred Picoseconds', C. T. White, D. H. Robertson, **M. L. Elert**, and D. W. Brenner, APS National Meeting, Indianapolis, IN, March 16-20, 1992 [Bull. Am. Phys. Soc. **37**, 361 (1992)].
34. 'Molecular Dynamics Simulations of Chemically Sustained Shock Waves', D. H. Robertson, C. T. White, D. W. Brenner, and **M. L. Elert**, American Chemical Society National Meeting, San Francisco, CA, April 6-10, 1992.
35. 'Molecular Dynamics Simulations of Chemically Sustained Shock Waves', C. T. White, D. H. Robertson, **M. L. Elert**, and D. W. Brenner, American Physical Society National Meeting, Seattle, WA, March 22-26, 1993 [Bull. Am. Phys. Soc. **38**, 796 (1993)].
36. 'Molecular Dynamics of Void Collapse Mechanisms in Shocked Media', J. W. Mintmire, D. H. Robertson, **M. L. Elert**, D. W. Brenner, and C. T. White, Topical Group on Shock Compression of Condensed Matter and the International Association for the Advancement of High Pressure Science and Technology (AIRAPT) – Joint Meeting, Colorado Springs, CO, June 28 – July 2, 1993.
37. 'Molecular Dynamics Study of the Reaction Zone in Condensed-Phase Detonation', **M. L. Elert**, D. H. Robertson, and C. T. White, American Physical Society National Meeting, San Jose, CA, March 20-24, 1995 [Bull. Am. Phys. Soc. **40**, 706 (1995)].
38. 'Molecular Dynamics Study of Reaction Zone Properties in Chemically Sustained Shock Waves', **M. L. Elert**, D. H. Robertson, J. J. C. Barrett, and C. T. White, American Physical Society Conference on Shock Compression of Condensed Matter, Seattle, WA, August 13-18, 1995.

## **Mark L. Elert**

---

### **Papers presented (cont'd.)**

39. 'Molecular Dynamics Study of Chemistry from Strong Shock Waves Interacting with Voids', C. T. White, J. J. C. Barrett, J. W. Mintmire, **M. L. Elert**, and D. H. Robertson, American Physical Society Conference on Shock Compression of Condensed Matter, Seattle, WA, August 13-18, 1995.
40. 'Effects of Nanoscale Voids on the Sensitivity of Model Energetic Materials', C. T. White, J. J. C. Barrett, J. W. Mintmire, **M. L. Elert**, and D. H. Robertson, Materials Research Society Meeting, Boston, MA, November 27 – December 1, 1995.
41. 'Molecular Dynamics Study of the Effect of Varying Exothermicity on the Properties of Condensed-Phase Detonation', **M. L. Elert**, D. H. Robertson, and C. T. White, Materials Research Society Meeting, Boston, MA, November 27 – December 1, 1995.
42. 'Effects of Crystalline Defects on the Initiation to Detonation Process in Model Energetic Materials', J. J. C. Barrett, D. H. Robertson, **M. L. Elert**, and C. T. White, Gordon Research Conference on Energetic Materials, New Hampton School, NH, June 16-21, 1996.
43. 'Molecular Dynamics Investigation of the Effects of Variation in Energy Release on Detonation Initiation', **M. L. Elert**, J. J. C. Barrett, D. H. Robertson, and C. T. White, American Physical Society Conference on Shock Compression of Condensed Matter, Amherst, MA, July 27 – August 1, 1997 [Bull. Am. Phys. Soc. **42**, 1514 (1997)].
44. 'Detonation Hugoniot for Ozone from Molecular Dynamics Simulation', J. J. C. Barrett, D. H. Robertson, **M. L. Elert**, and C. T. White, American Physical Society Conference on Shock Compression of Condensed Matter, Amherst, MA, July 27 – August 1, 1997 [Bull. Am. Phys. Soc.; **42**, 1514 (1997)].
45. 'Self-Similar Behavior from Molecular Dynamics Simulations of Detonations', D. H. Robertson, J. J. C. Barrett, **M. L. Elert**, and C. T. White, American Physical Society Conference on Shock Compression of Condensed Matter, Amherst, MA, July 27 – August 1, 1997 [Bull. Am. Phys. Soc. **42**, 1514 (1997)].
46. 'Detonation Hugoniots from Molecular Dynamics Simulations', D. R. Swanson, J. W. Mintmire, **M. L. Elert**, C. T. White, and D. H. Robertson, American Physical Society National Meeting, Los Angeles, CA, March 16-20, 1998.
47. 'Molecular Dynamics Simulation of Shock-Induced Chemistry in Acetylene', **M. L. Elert**, D. R. Swanson, and C. T. White, American Physical Society Conference on Shock Compression of Condensed Matter, Snowbird, Utah, June 27 – July 2, 1999.
48. 'Critical Widths in Molecular Dynamics Simulations of Detonations', C. T. White, D. H. Robertson, D. R. Swanson, and **M. L. Elert**, American Physical Society Conference on Shock Compression of Condensed Matter, Snowbird, Utah, June 27 – July 2, 1999.
49. 'Detonation Hugoniots Produced by Piston-Driven Simulations', D. R. Swanson, **M. L. Elert**, and C. T. White, American Physical Society Conference on Shock Compression of Condensed Matter, Snowbird, Utah, June 27 – July 2, 1999.
50. 'Molecular Dynamics Modeling of Impact-Induced Shock Waves in Hydrocarbons', **M. L. Elert**, Sergey Zybin, and C. T. White, American Physical Society Conference on Shock Compression of Condensed Matter, Atlanta, Georgia, June 24-29, 2001.

## **Mark L. Elert**

---

### **Papers presented (cont'd.)**

51. 'Atomistic Modeling of Orientation Dependence of Shock Wave Properties in Diamond', Sergey Zybin, **M. L. Elert**, Vasilii Zhakhovskii, and C. T. White, American Physical Society Conference on Shock Compression of Condensed Matter, Atlanta, Georgia, June 24-29, 2001.
52. 'Molecular Dynamics Modeling of Non-Reacting Shock Waves in Hydrocarbon Molecular Crystals', Sergey Zybin, **M. L. Elert**, and C. T. White, American Physical Society National Meeting, Indianapolis, Indiana, March 18-22, 2002.
53. 'Molecular Dynamics Simulation of Shock-Induced Polymerization of Hydrocarbons', **M. L. Elert**, Sergey Zybin, and C. T. White, American Physical Society National Meeting, Indianapolis, Indiana, March 18-22, 2002.
54. 'Modeling of Shock Wave Effects in Carbon and Hydrocarbon Systems', **M. L. Elert**, S. V. Zybin, and C. T. White, Gordon Research Conference on Energetic Materials, Tilton, New Hampshire, June 16-21, 2002.
55. 'Modeling Shock-Induced Chemistry in Carbon and Hydrocarbon Systems with a Reactive Empirical Potential', **M. L. Elert**, S. V. Zybin, and C. T. White, CECAM (European Centre for Atomic and Molecular Computations) Workshop, 'Upscaling from *ab initio* to Molecular Dynamics: Interatomic Potentials and Hybrid Methods', Lyon, France, July 8-12, 2002.
56. 'Orientation Dependence of Shock-Induced Plasticity and Chemistry in Diamond', C. T. White, S. V. Zybin, and **M. L. Elert**, TMS Annual Meeting, San Diego, California, March 2-6, 2003.
57. 'Oscillatory Structure of Elastic Precursor in Shocked Crystalline Solids: A Molecular Dynamics Study', S. V. Zybin, V. Zhakhovskii, **M. L. Elert**, and C. T. White, American Physical Society National Meeting, Austin, Texas, March 3-7, 2003.
58. 'Shock-Induced Plasticity and Chemistry in Diamond: Orientation and Shock Strength Dependence', S. V. Zybin, **M. L. Elert**, and C. T. White, American Physical Society National Meeting, Austin, Texas, March 3-7, 2003.
59. 'Shock-Induced Chemistry in Aromatic Hydrocarbons', **M. L. Elert**, S. V. Zybin, and C. T. White, APS Topical Conference on Shock Compression of Condensed Matter, Portland, Oregon, July 20-25, 2003.
60. 'Molecular Dynamics Study of Non-Reacting Shock Waves in Hydrocarbon Molecular Crystals', S. V. Zybin, **M. L. Elert**, and C. T. White, APS Topical Conference on Shock Compression of Condensed Matter, Portland, Oregon, July 20-25, 2003.
61. 'Molecular Dynamics Studies of Orientation Dependence of Shock Structure in Solids', S. V. Zybin, **M. L. Elert**, and C. T. White, APS Topical Conference on Shock Compression of Condensed Matter, Portland, Oregon, July 20-25, 2003.
62. 'Molecular Dynamics of Shock Waves and Detonation', **M. L. Elert**, Sigma Xi Lecture, USNA Chapter, December 5, 2003.
63. 'Orientation Dependence of Reactive and Nonreactive Shock Waves in Anthracene by Molecular Dynamics', **M. L. Elert**, S. V. Zybin, and C. T. White, American Physical Society National Meeting, Montreal, Quebec, Canada, March 22-26, 2004.
64. 'Instability and Deformation of Diamond Under Shock Loading via Atomistic Modeling', S. V. Zybin, I. I. Oleynik, **M. L. Elert**, and C. T. White, International Conference on New Models and Hydrocodes for Shock Wave Processes, College Park, Maryland, May 16-20, 2004.

## **Mark L. Elert**

---

### **Papers presented (cont'd.)**

65. 'Classical and Quantum Dynamics of Energy Transfer under Shock Conditions', R. C. Mowrey, **M. L. Elert**, and C. T. White, APS Topical Conference on Shock Compression of Condensed Matter, Baltimore, Maryland, July 31 – August 5, 2005.
66. 'Nanoscale Molecular Dynamics Simulation of Shock Compression of Silicon', D. Lovelady, I. I. Oleynik, S. V. Zybin, **M. L. Elert**, and C. T. White, APS Topical Conference on Shock Compression of Condensed Matter, Baltimore, Maryland, July 31 – August 5, 2005.
67. 'Shear Stresses in Shock-Compressed Covalent Solids', I. I. Oleynik, D. Lovelady, S. V. Zybin, **M. L. Elert**, and C. T. White, APS Topical Conference on Shock Compression of Condensed Matter, Baltimore, Maryland, July 31 – August 5, 2005.
68. 'Molecular Dynamics Simulation of Shock Compression of Silicon', M. Ladanov, I. I. Oleynik, S. V. Zybin, **M. L. Elert**, and C. T. White, American Physical Society National Meeting, Baltimore, Maryland, March 13-17, 2006.
69. 'Quantum Dynamics of Energy Transfer under Shock Conditions', R. C. Mowrey, **M. L. Elert**, and C. T. White, American Physical Society National Meeting, Baltimore, Maryland, March 13-17, 2006.
70. 'Shock-Induced Chemical Reactions of Polycyclic Aromatic Hydrocarbons', **M. L. Elert**, S. V. Zybin, S. M. Revell, and C. T. White, American Physical Society National Meeting, Baltimore, Maryland, March 13-17, 2006.
71. 'Atomic Simulation of Energetic Materials', **M. L. Elert**, Second Eglin Symposium on Nano Energetics, Shalimar, Florida, March 22-23, 2006.
72. 'Anomalous Elastic Response of Diamond Single Crystals to Shock Compression', K. McLaughlin, M. Y. Ladanov, I. I. Oleynik, S. V. Zybin, **M. L. Elert**, and C. T. White, American Physical Society National Meeting, Denver, Colorado, March 5-9, 2007.
73. 'Molecular Dynamics Simulations of an Anomalous Response of Diamond to Shock Compression', K. McLaughlin, I. I. Oleynik, S. V. Zybin, **M. L. Elert**, and C. T. White, APS Topical Conference on Shock Compression of Condensed Matter, Waikoloa, Hawai'i, June 24-29, 2007.