

Damian Gregory Allis, Ph.D.

Research Assistant Professor, Department of Chemistry, Syracuse University

work: Syracuse University, 1-014 CST, Syracuse, NY, USA 13244
home: 313 East Willow Street Apt. 501, Syracuse, NY, USA 13203
web: www.somewhereville.com (or www.damianallis.com)
email: damian@somewhereville.com (1st), dgallis@syr.edu (2nd),
somewhereville@gmail.com (3rd)

home: (315) 559-4737
office: (315) 443-2067, **fax:** (315) 443-4070
[aim](#)/[facebook](#)/[flickr](#)/[friendster](#)/[gtalk](#)/[linkedin](#)/
[myspace](#)/[skype](#)/[twitter](#)/[google+](#):
somewhereville

RESEARCH DESCRIPTION (Publication Summary and Current Research)

Computational quantum chemistry; molecular nanotechnology; the design and simulation of molecules and nanostructures, molecular-based materials for molecular electronics and nonlinear optical materials applications, nanostructures from molecular building blocks and biomimetic principles; mechanosynthetic approaches in advanced molecular manufacturing; the property prediction of solid-state materials from density functional theoretical approaches; inelastic neutron scattering vibrational theory and calculation; computational drug design and modeling interaction pathways; molecular modeling, vibrational properties, and predictive modeling tools for crystal polymorphism; the simulation of internal/external vibrations and conformational changes observed by terahertz (THz) spectroscopy; electronic structure theory of inorganic clusters and organometallic coordination complexes; molecular dynamics simulations and reduced model development of DNA-based nanostructures; computational design principles, property prediction and evaluation in bioconjugate chemistry; molecular mechanics/dynamics force field development; extensive background in computer hardware and software, including systems design, administration, security, cluster assembly, parallel computing platforms, national computing facility utilization (NCSA) and distributed computing, maintenance, graphics design, and web development.

EDUCATION

Syracuse University (Aug 1998 – Oct 2004), Syracuse, New York, USA

Graduate Fellow, Doctor of Philosophy, Physical Inorganic/Computational Quantum Chemistry

Thesis : **Computational Quantum Chemistry In Initial Designs And Final Analyses**

Thesis Defense: October 15, 2004, 30 GPA credits, *summa cum laude*

Advisor : Bruce S. Hudson, Ph.D. (2001-2004)

The comparison of theory and experiment in the inelastic neutron scattering vibrational structure of multi-molecular systems and periodic molecular arrays (crystals), focusing on hydrogen-bonded networks and organic crystal engineering; the application of periodic density functional theory to the study of electronic structure in the solid state, including molecular crystals, periodic lattices, molecular density-of-states, and polymorphism/crystal structure prediction.

Advisor : James T. Spencer, Ph.D. (1998-2004)

Molecular building block and biomimetic approaches to nanostructure design and fabrication; electronic structure theory of main group clusters, emphasizing their interactions with organic species for molecular electronics and nonlinear optical materials applications.

Departmental Research : Jon Zubieta, Ph.D. and Karin Ruhlandt, Ph.D. (2002-2004)

Theory and modeling of isomerization/rearrangement pathways of solid-state materials formed via the hydrothermal-based inorganic-organic hybrid chemistry of inorganic oxides, with specific focus on the octamolybdate class of isomers (Zubieta); computational molecular biology and transition metal radiopharmaceutical drug design via classical Molecular Mechanics/Molecular Dynamics simulations (Zubieta, Molecular Insight, Inc.); quantum chemical studies of structure and stability among the heavy alkali organometallic complexes with emphasis on the elucidation of crystal morphology from quantum chemical approaches (Ruhlandt).

Syracuse University (Aug 1994 – May 1998), Syracuse, New York, USA

Bachelor of Science with Honors, Chemistry, May 1998, *magna cum laude*, 156/120 credits

SELECTED CONTENT, HONORS AND ORGANIZATIONS

Invited Essays, Interviews, Slidecasts, Free Press, Talks

Invited Lecture: Allis D.G. When Mechanical Engineering and Quantum Mechanics Meet - Using Computational Chemistry to Predict a Future for Molecular Manufacturing. A*STAR - Institute of Materials Research and Engineering (IMRE) Workshop on Atom Technology and its Applications, Singapore, June 10, 2010.

Syracuse University Project Advance Spring Meeting, Syracuse, NY, April 27, 2010 and Lubin House, New York City, NY, May 13, 2010.

Invited Lecture: Allis D.G. Vitamin B₁₂ As A Tool For Drug Delivery; Building Atom-By-Atom - Computational Studies In Mechanosynthesis. Syracuse University Project Advance Spring Meeting, Syracuse, NY, April 27, 2010 and Lubin House, New York City, NY, May 13, 2010.

Interview: Syracuse University Partners With Serum Institute Of India To Develop Vaccines For Children. Syracuse University Arts and Sciences Press Release, 2008.

Slidecast: Single-Atom Manipulation and the Chemistry of Mechanosynthesis. NanoScienceWorks, Taylor & Francis (www.nanoscienceworks.org/slidecast), December, 2007.

Guest Essay: Exploring the Productive Nanosystems Roadmap, Center for Responsible Nanotechnology Newsletter (www.crmno.org), October, 2007.

Interview: Solid-State Modeling of the Terahertz Spectrum of the Explosive HMX, Accelrys case study (www.accelrys.com), August, 2006.

Interview: Olson S. An Interview with Damian Gregory Allis. for Nanotech.biz (www.nanotech.biz), November, 2005.

Interview: Caponi K.A. Towards Computing Crystal Forms. Access Magazine, National Center for Supercomputing Applications, Vo. 17, No. 1, Spring 2004.

Invited Lecture: Allis D.G. Single Atom Manipulation and the Chemistry of Mechanosynthesis. Productive Nanosystems: Launching the Technology Roadmap, Arlington, VA USA October 9-10, 2007.

Invited Lecture: Allis D.G. Chemical Origins of Solid-State Terahertz Spectra. DIA/NGA Community Academic Summit, Williamsburg VA June 11-13, 2007.

Lecture: Allis D.G. Novel Imaging and Spectroscopy Technologies - Terahertz Detector Device Deployment and Theory for Terahertz Biomolecular And Molecular Threat Agent Spectroscopy, IC Postdoctoral Research Fellowship Colloquium, Chantilly, VA, April 30 - May 3, 2007.

Invited Lecture: Allis D.G. Nanosystem Simulation and Design for Molecular Manufacturing. Department of Mechanical and Aeronautical Engineering, Clarkson University, Potsdam, NY, February 27, 2007.

Keynote Lecture: Allis D.G. Nanotechnology and Molecular Manufacturing. Ibero-American Conference for University and College Presidents: Global Workforce Trends and Emerging Technologies, Advanced Technology Center ATC, Alamo Community College District, San Antonio, Texas September 18-20, 2006.

Invited Lecture: Allis D.G. Computational Chemistry for the Next 6 Months and 50 (or so) Years: Quantum Theory Applications in Homeland Security and Molecular Manufacturing. Syracuse University Project Advance Spring Meeting, Syracuse, NY,

March 22, 2006 and Lubin House, New York City, NY, May 27, 2006.

Lecture: Allis D.G. The Design of Carbon Nanotube-Based Dative Structures from Supramolecular Principles. Foresight Institute Tenth Conference on Nanotechnology, Bethesda, MD, October 10-12, 2002.

Invited Lecture: Allis D.G. An Introduction to Computer Aided Chemistry and Nanomechanical Design Using CAChe. Syracuse University Project Advance Spring Meeting, Lubin House, New York City, NY, May 18-19, 2000.

Selected Honors Director of Central Intelligence Postdoctoral Research Fellow (2005-2007), Marquis Who's Who in the World, in Science and Engineering, and in America, Foresight Distinguished Student Award in Nanotechnology (2004), Syracuse University All-University Graduate Fellowship (1998-2001, three year appointment), Who's Who Among Students in America's Colleges and Universities (1998), Phi Beta Kappa (1998), Syracuse University Merck Index Award (1998), Golden Key National Honors Society (1996), Phi Eta Sigma (1995), Syracuse University Honors Program (1994-8), Syracuse University Dean's Scholar (1994-8, all semesters), John Philip Sousa Award (Jamesville-DeWitt School District, 1994)

Affiliations, Organizations, Professional Activities Chinese Optics Letters (Reviewer 2011-), Journal of Molecular Structure (Reviewer 2010-), Materials Chemistry and Physics (Reviewer 2009-), Neutron Scattering Society Of America (Member 2009-), Lifeboat Foundation (Nanotechnology and Chemistry Advisory Board Member 2007-), International Society of Nanoscale Science, Computation, and Engineering (Member 2007-), Technology Alliance of Central New York (TACNY, Organizational Affiliate, Member 2007-), Chemical Physics Letters (Reviewer 2007-), Technology Roadmap for Productive Nanosystems (Contributing Editor and Working Group Member 2005-2007), Inorganic Chemistry Communications (Reviewer 2005-), Molecular Engineering Research Institute (Member 2004-2008), The Syracuse Astronomical Society (Board of Directors 2003- and President 2007-), American Association for the Advancement of Science (Member 1997-), The Foresight Institute (Member 1997-), The Planetary Society (Member 1996-), American Chemical Society (Member 1995-)

Molecular Graphics In-Print (Excluding Web-Only Content) Journal Of Physical Chemistry A (Cover, November 2010), Molecular Biosystems (Inside Cover, August 2010), Journal of Organic Chemistry (Cover, May 2010), Clinical Chemistry (Cover, April 2010), ChemMedChem (Cover, March 2009), ChemMedChem (Cover, December 2007), Technology Roadmap for Productive Nanosystems (Content, 2008), The Future for Nanoscience and Nanotechnology, RSC and IOP (Content, 2008), Productive Nanosystems: Launching the Technology Roadmap (Cover, 2007), "Erlebnis Wissenschaft" Wiley-VCH Book Series (Content, 2007), Nanotechnologien für die Optische Industrie, www.hessen-nanotech.de (Content, 2007), Großes Netzwerk für Kleine Teilchen Aerosolforschung in der GSF (Content, 2007), Accelrys Chemical Case Study (Content, 2006), Tennessee's Business (Cover and Content, Vol. 15, 2006), Revista Latitude (Content, 2006), *Nanoaventura*, Museu Exploratorio de Ciências de Campinas, Instituto Sangari, (Content, 2005)

CURRENT RESEARCH AND PROFESSIONAL POSITION

Syracuse University, Syracuse, New York, USA (2007-)

Research Assistant Professor, Department of Chemistry, Departmental and External Collaborative Computational Chemistry Research

AptaMatrix, Inc. (formerly Orthosystems, Inc.), Syracuse, New York, USA (2010-)

Bioinformatics, Computational Modeling and Web Development

Nanofactory Collaboration, www.molecularassembler.com/Nanofactory/ (2006-)

Independent Research, Multiple Ongoing Academic and Industrial Research Projects

SELECTED PAST RESEARCH AND PROFESSIONAL POSITIONS

Nanorex, Inc., www.nanorex.com, Bloomfield Hills, Michigan, USA (2004-2008)

Senior Scientist and former Scientific Advisory Board Member

- Molecular CAD-based structural DNA nanotechnology software design and force field development
- Quantum/classical nanostructure modeling and software design tools for molecular manufacturing
- nanoEngineer-1 v1.0.0, 2008 winner, Products Category, Nanotech Briefs "Nano50"

Nanohive@HOME, www.nanohive-1.org (February – May, 2007, defunct 2008)

Project Developer, Scientific Advisor, and Content Provider

- BOINC-based distributed computing system (developed by Brian Helfrich) for nanostructure simulations
- General quantum/classical simulation tool for conformational and structural rearrangement searches
- Tooltip Failure Mode Search Project peaked at an unadvertised 3 teraFLOPS (see paper Ref. 42)

Molecular Insight Pharmaceuticals, Inc., Cambridge, Massachusetts, USA (2003-2007)

Consultation Position in Computational Radiopharmaceutical Design, www.molecularinsight.com

- Biomolecular modeling and molecular dynamics simulations of novel synthetic radiopharma targets
- Involved in new target planning sessions and responsible for AMBER/GROMOS force field development
- First design study (biotin-based analogues for ReCO_3 complexation) is paper Ref. 14 (Bioconj. Chem.)

ICPDRFP/CIA, Washington, D.C. (September 2005 - September 2007, 2 Year Appointment)

Director of Central Intelligence Postdoctoral Research Fellow with Dr. Timothy Korter

- Theory and modeling of molecular phenomena observed in solid-state terahertz (THz) spectroscopy
- Several papers and presentations of results relevant to threat agent/drug identification and polymorphism
- First publication (Paper Ref. 12) highlighted in Science and Chemical and Engineering News

Nanoworks Incorporated, Fayetteville, New York, USA (1999-2002)

Senior Theoretician, Nanosystems Design and Simulation, Photonic and Thin Film Materials

- Principle Investigator for BMDO 2000 Phase I SBIR: Optical Computing & Optical Signal Processing
- Theory and design of novel molecular nonlinear optical materials for use in optical-based technologies
- Molecular modeling studies served as the basis for experimental work described in Patents (see below) and several publications and presentations

Department of Chemistry, Syracuse University, Syracuse, New York, USA (1996-8)

Undergraduate Researcher, Research Experience for Undergraduates (REU)

- Photolytic studies of borane clusters and aromatic systems by experimental and theoretical methods
- Theoretical studies of the photoisomerization chemistry of rhodium- and manganese-containing boranes

Syracuse Research Corporation/VA Hospital, Syracuse, New York, USA (1995-7)

Biological Sciences Student Trainee, Laboratory Technician for Brad C. Motter, Ph.D.

- Responsible for the design and fabrication of multi-channel tetrode hyperdrives, used chronically in the recording of activity in the mammalian cerebellum V1, V2, and V4 regions
- Surgical assistant, computer interface and protocols developer for device data collection

Northeast Parallel Architectures Center, Syracuse, New York, USA (1994-7)

Internet and Database Development for www.csir.org (website defunct, 2001)

- Responsible for processing and cataloging of software submissions for Chemistry Software and Information Resources (www.csir.org), an online chemistry software information database.
- Developed new GUI and HTML protocols to work with the new site requirements, including the restructuring of the existing databases for IEEE compliance.

PUBLICATIONS (Peer-Reviewed Only)

43. Clardy S., Allis D.G., Fairchild T.J., and Doyle R. "Vitamin B₁₂ in Drug Delivery: Breaking Through the Barriers to a B12 Bioconjugate Pharmaceutical." Expert Opinion on Drug Delivery, 8, 1 (2011) 127-140, DOI:10.1517/17425247.2011.539200.

42. Allis D.G., Helfrich B., Freitas Jr., R. A., and Merkle R. C. "Analysis of Diamondoid Mechanosynthesis Tooltip Pathologies Generated via a Distributed Computing Approach." *Journal of Computational and Theoretical Nanoscience*, 8 (2011) 1139-1161, DOI:10.1166/jctn.2011.1792.
41. Allis D.G., Fairchild T.J., and Doyle R. "The Binding of Vitamin B12 to Transcobalamin(II); Structural Considerations for Bioconjugate Design – a Molecular Dynamics Study." *Molecular Biosystems*, 6 (2010) 1611-1618. DOI:10.1039/c003476b.
40. Buchanan W.D., Allis D.G., and Ruhlandt-Senge S. "Synthesis and Stabilization – Advances in Organoalkaline Earth Metal Chemistry." *Chemical Communications*, 46 (2010) 4449-4465. DOI:10.1039/C002600J.
39. Hudson M.R., Allis D.G., and Hudson B.S. "The Vibrational Spectrum of Parabanic Acid by Inelastic Neutron Scattering Spectroscopy and Simulation by Solid-State DFT." *Journal of Physical Chemistry A*, 114(10) (2010) 3630-3641. DOI: 10.1021/jp9114095.
38. Hakey P.M., Allis D.G., Hudson M.R., Ouellette W., and Korter T.M. "Terahertz Spectroscopic Investigation of S-(+)-Ketamine Hydrochloride and Vibrational Assignment by Density Functional Theory." *Journal of Physical Chemistry A*, 114(12) (2010) 4364-4374. DOI: 10.1021/jp910861m.
37. Hakey P.M., Hudson M.R., Allis D.G., Ouellette W., and Korter T.M. "Examination of Phencyclidine Hydrochloride via Cryogenic Terahertz Spectroscopy, Solid-State Density Functional Theory, and X-Ray Diffraction." *Journal of Physical Chemistry A*, 113(46) (2009) 13013-13022. DOI:10.1021/jp907083u.
36. Hudson M.R., Allis D.G., Ouellette W., and Hudson B.S. "Low-Temperature X-ray Structure Determination and Inelastic Neutron Scattering Spectroscopic Investigation of L-Alanine Alaninium Nitrate, a Homologue of a Ferroelectric Material." *Physical Chemistry Chemical Physics*, 11(41) (2009) 9474-9483. DOI:10.1039/B905070A.
35. Motley T.L., Allis D.G., and Korter T.M. "Investigation of Crystalline 2-Pyridone Using Terahertz Spectroscopy and Solid-State Density Functional Theory." *Chemical Physics Letters* 478(4-6) (2009) 166-171. DOI:10.1016/j.cplett.2009.07.078.
34. Hudson M.R., Allis D.G., Ouellette W., Hakey P.M., and Hudson B.S. "The Low-Temperature X-ray Structure, Raman and Inelastic Neutron Scattering Vibrational Spectroscopic Investigation of the Non-centrosymmetric Amino Acid Salt Glycine Lithium Sulfate." *Journal of Molecular Structure*, 934(1-3) (2009) 138-144. DOI:10.1016/j.molstruc.2009.06.033.
33. Hakey P.M., Allis D.G., Hudson M.R., Ouellette W., and Korter T.M. "An Investigation of (1R,2S)-(-)-Ephedrine Using Solid-State Density Functional Theory and Cryogenic Terahertz Spectroscopy." *ChemPhysChem* 10(14) (2009) 2434-2444. DOI:10.1002/cphc.200900293.
32. Hudson M.R., Allis D.G., and Hudson B.S. "The Inelastic Neutron Scattering Spectrum Of Nicotinic Acid And Its Assignment By Solid-State Density Functional Theory." *Chemical Physics Letters*, 473 (1-3) (2009) 81-87. DOI:10.1016/j.cplett.2009.03.052.
31. Hakey P.M., Allis D.G., Ouellette W., and Korter T.M. "The Cryogenic Terahertz Spectrum Of (+)-Methamphetamine Hydrochloride And Assignment Using Solid-State Density Functional Theory." *Journal of Physical Chemistry A*, 113(17) (2009) 5119–5127. DOI:10.1021/jp810255e.
30. Hakey P.M., Allis D.G., Hudson M.R., and Korter T.M. "Density Functional Dependence In The Theoretical Analysis Of The Terahertz Spectrum Of The Illicit Drug MDMA (Ecstasy)." *IEEE Sensors Journal*, *accepted*.
29. Petrus A.K., Allis D.G., Smith R.P., Fairchild T.J., and Doyle R.P. "Exploring The Implications Of Vitamin B12 Conjugation To Insulin On Insulin Receptor Binding And Cellular Update." *ChemMedChem*, 4(3) (2009) 421-426. DOI:10.1002/cmcd.200800346.

28. Rivera S., Allis D.G., and Hudson B.S. "Importance Of Vibrational Zero-Point Energy Contribution To The Relative Polymorph Energies Of Hydrogen-Bonded Species." *Crystal Growth and Design*, 8(11) (2008) 3905–3907. DOI:10.1021/cg800524d.
27. Fedor A.M., Allis D.G., and Korter T.M. "The Terahertz Spectrum And Quantum Chemical Assignment Of 2,2'-Bithiophene In Cyclohexane." *Vibrational Spectroscopy*, 49(2) (2009) 124-132. DOI:10.1016/j.vibspec.2008.06.001.
26. Allis D.G., Hakey P.M., and Korter T.M. "The Solid-State Terahertz Spectrum of MDMA (Ecstasy) – A Unique Test for Molecular Modeling Assignments." *Chemical Physics Letters*, 463 (2008) 353-356. DOI:10.1016/j.cplett.2008.08.024.
25. O'Leary D.J., Allis D.G., Hudson B.S., James S., Morgera K.B., and Baldwin J.E. "Vicinal Deuterium Perturbations on Hydrogen NMR Chemical Shifts in Cyclohexanes." *Journal of the American Chemical Society*, 130(41) (2008) 13659-13663. DOI:10.1021/ja802903a.
24. Allis D.G., Zeitler J.A., Taday P.F., and Korter T.M. "Theoretical Analysis of the Solid-State Terahertz Spectrum of the High Explosive RDX." *Chemical Physics Letters*, 463 (2008) 84-89. DOI:10.1016/j.cplett.2008.08.014.
23. Armatas N.G., Allis D.G., Prosvirin A., Carnutu G., O'Connor C.J., Dunbar K., and Zubieta J. "Molybdophosphonate Clusters As Building Blocks In The Oxomolybdate-Organodiphosphonate/Cobalt(II)-Organoimine System: Structural Influences Of Secondary Metal Coordination Preferences And Diphosphonate Tether Lengths." *Inorganic Chemistry*, 47 (2008) 3, 832 -854. DOI:10.1021/ic701573r.
22. Alexander J.S., Allis D.G., Teng W., and Ruhlandt-Senge K. "Alkali Metal Diphenylmethanides: Synthetic, Computational and Structural Studies." *Chemistry - A European Journal*, 13 (2007) 35, 9899-9911. DOI:10.1002/chem.200700763.
21. Allis D.G., Fedor A.M., Korter T.M., Bjarnason J.E., and Brown E.R. "Assignment Of The Lowest-Lying THz Absorption Signatures In Biotin And Lactose Monohydrate By Solid-State Density Functional Theory." *Chemical Physics Letters*, 440 (2007) 203-209. DOI:10.1016/j.cplett.2007.04.032. Reprint in *Journal of Intelligence Community Research and Development*, 2007.
20. Freitas Jr. R.A., Allis D.G., and Merkle R. "Horizontal Ge-Substituted Polymantane-Based C2 Dimer Placement Tooltip Motifs for Diamond Mechanosynthesis." *Journal of Computational and Theoretical Nanoscience*, 4 (2007) 433-442. DOI:10.1166/jctn.2007.004.
19. Allis D.G. and Korter T.M. "Development Of Computational Methodologies for the Prediction And Analysis of Solid-State Terahertz Spectra." *International Journal of High Speed Electronics and Systems*, 17(2) (2007) 193-212. DOI:10.1142/S0129156407004436. Reprint in *Journal of Intelligence Community Research and Development*, 2007.
18. Teng W., Allis D.G., and Ruhlandt-Senge K. "Synthetic, structural and theoretical investigations of alkali metal germanium hydrides - contact molecules and separated ions." *Chemistry - A European Journal*, 13(4) (2006) 1309-1319. DOI:10.1002/chem.200601073.
17. Allis D.G. "Understanding the Chemical Origins of Terahertz Spectra." *Journal of Intelligence Community Research and Development*. Includes reprints of Pubs. 15 and 18.
16. Allis D.G. and Korter T.M. "Theoretical Analysis of the Terahertz Spectrum of the High Explosive PETN." *Chemphyschem: A European Journal of Chemical Physics and Physical Chemistry*, 7(11) (2006) 2398-408. DOI:10.1002/cphc.200600456.
15. Allis D.G., Prokhorova D.A., Fedor A.M., and Korter T.M. "First Principles Analysis of the Terahertz Spectrum of PETN." *Proceedings of SPIE-The International Society for Optical Engineering*, 6212 (2006) (Terahertz for Military and Security Applications IV) 62120F/1-62120F/11. DOI:10.1117/12.665787.

14. James S., Maresca K.P., Allis D.G., Valliant J.F., Eckelman W., Babich J.W., and Zubieta J. "Extension Of The Single Amino Acid Chelate Concept (SAAC) To Bifunctional Biotin Analogues For Complexation Of The $M(\text{CO})_{3+1}$ Core ($M = \text{Tc}$ And Re): Syntheses, Characterization, Biotinidase Stability And Avidin Binding." *Bioconjugate Chemistry*, 17 (2006) 579-589. DOI:10.1021/bc050297w.
13. Allis D.G. and Hudson B.S. "The Inelastic Neutron Scattering Spectrum of $\text{Cs}_2[\text{B}_{12}\text{H}_{12}]$: Reproduction of its Solid-State Vibrational Spectrum by Periodic DFT." *Journal of Physical Chemistry A*, 110 (2006) 3744-3749. DOI:10.1021/jp055285m.
12. Allis D.G., Prokhorova D.A., and Korter T.M. "Solid-State Modeling of the Terahertz Spectrum of the High Explosive HMX." *Journal of Physical Chemistry A*, 110 (2006) 1951-1959. DOI:10.1021/jp0554285.
11. Hudson B. S., Allis. D. G., Parker S. F., Ramirez-Cuesta, A. J., Hermanc, H., and Prinzbach, H. "Infrared, Raman and inelastic neutron scattering spectra of dodecahedrane: An Ih molecule in Th site symmetry." *Journal of Physical Chemistry A*, 109 (2005) 3418 -3424. DOI:10.1021/jp0503213.
10. Allis D. G. and Drexler K. E. "Design and Analysis of a Molecular Tool for Carbon Transfer in Mechanosynthesis." *Journal of Computational and Theoretical Nanoscience*, 2 (2005) 45-55. DOI:10.1166/jctn.2005.003.
9. Hudson B. S., Braden D. A., Allis D. G., Jenkins T., Baronov S., Middleton C., Withnall R., and Brown C. M. "The Crystalline Enol of 1,3-Cyclohexanedione and its Complex with Benzene: Vibrational Spectra, Simulation of Structure and Dynamics and Evidence for Cooperative Hydrogen Bonding." *Journal of Physical Chemistry A*, 108 (2004) 7356-7363. DOI:10.1021/jp048613b.
8. Allis D.G., Kosmowski M.E., and Hudson B.S. "The Inelastic Neutron Scattering spectrum of $\text{H}_3\text{B}:\text{NH}_3$ and the Reproduction of Its Solid-State Features by Periodic DFT." *Journal of the American Chemical Society*, 126(25) (2004) 7756-7757. DOI:10.1021/ja048215m.
7. Allis D.G., Burkholder E., and Zubieta J. "A New Octamolybdate: Observation of the theta-Isomer in $[\text{Fe}(\text{tpyprz})_2]_2[\text{Mo}_8\text{O}_{26}]_3 \cdot 7\text{H}_2\text{O}$. (tpyprz = tetra-2-pyridylpyrazine)." *Polyhedron*, 23(7) (2004) 1145-1152. DOI:10.1016/j.poly.2004.01.011.
6. Allis D.G., Prinzbach H., and Hudson B.S. "Inelastic Neutron Scattering Spectra of Pagodane: Experiment and DFT Calculations." *Chemical Physics Letters*, 386 (2004) 356-363. DOI:10.1016/j.cplett.2004.01.076.
5. Allis D.G. and Hudson B.S. "Inelastic Neutron Scattering Spectra of NaBH_4 and KBH_4 : Reproduction of Anion Mode Shifts via Periodic DFT." *Chemical Physics Letters*, 385 (2004) 166-172 DOI:10.1016/j.cplett.2003.12.046.
4. Allis D.G., Rarig R.S., Burkholder E., and Zubieta J. "A Three-Dimensional Bimetallic Oxide Constructed from Octamolybdate Clusters and Copper-Ligand Cation Polymer Subunits. A Comment on the Stability of the Octamolybdate Isomers." *Journal of Molecular Structure*, 688 (2004) 11-31. DOI:10.1016/j.molstruc.2003.08.027.
3. Alexander J.S., Allis D.G., Hudson B.S., and Ruhlandt-Senge K. "An Examination of Metal-Ligand Binding Modes in Rubidium Diphenylmethanide." *Journal of the American Chemical Society*, 125(49) (2003) 15002-15003. DOI:10.1021/ja037201y.
2. Allis D.G. and Spencer J.T. "Polyhedral-Based Nonlinear Optical Materials. Part 2. Theoretical Investigation of Some New High Nonlinear Optical Response Compounds Involving Polyhedral Bridges with Charged Aromatic Donors and Acceptors." *Inorganic Chemistry*, 40 (2001) 3373-3380. DOI:10.1021/ic0007761.
1. Allis D.G. and Spencer J.T. "Polyhedral-Based Nonlinear Optical Materials. Part 1. Theoretical Investigation of Some New High Nonlinear Optical Response Compounds Involving Carboranes and Charged Aromatic Donors and Acceptors." *Journal of Organometallic Chemistry*, 614-615 (2000) 309-313. DOI:10.1016/S0022-328X(00)00589-1.

BOOKS AND CHAPTERS

6. Chapter: Allis D.G. and Korter T.M. Development Of Computational Methodologies for the Prediction And Analysis of Solid-State Terahertz Spectra. Selected Topics in Electronics and Systems – Vol. 46: Terahertz Science and Technology For Military and Security Applications, Woolard D.L., Jensen J.O., Hwu R.J., and Shur M.S. (Editors); World Scientific, 2007.

5. Roadmap: Productive Nanosystems: A Technology Roadmap. Drexler K.E., Randall J., Corchnoy S., Kawczak A., Steve M.L. (Editors), Soreff J., Allis D.G., Von Ehr J. (Contributing Editors), Battelle Memorial Institute and Foresight Nanotech Institute, 2007. Contributions include: Synthetic Chemistry, Mechanosynthesis, and Design and Modeling.

4. Chapter: Allis D.G. and Spencer J.T. Nanostructural Architectures from Molecular Building Blocks. CRC Handbook of Nanoscience, Engineering, and Technology, 2nd Edition, Goddard III W.A.; Lyshevski S.E.; Brenner D.W.; Iarfrate G.J. (Editors); Francis and Taylor Publishers, 2007.

3. Book: Allis D.G. Computational Quantum Chemistry in Initial Designs and Final Analyses. Syracuse University, Syracuse, NY, USA, UMI No. DA3160378 (2004) 509 pp. Dissertation Abstracts Int., B 2005, 66(1), 293.

2. Chapter: Allis D.G. and Spencer J.T. Nanostructural Architectures from Molecular Building Blocks. CRC Handbook of Nanoscience, Engineering, and Technology, Goddard III W.A.; Lyshevski S.E.; Brenner D.W.; Iarfrate G.J. (Editors); CRC Press, 2002.

1. Chapter: Littger R.; Taylor J.; Rudd G.; Newlon A.; Allis D.G.; Kotiah S.; Spencer J.T. Thermal, Photochemical, and Redox Reactions of Borane and Metallaborane Clusters with Applications to Molecular Electronics Contemporary Boron Chemistry; Davidson M.G.; Hughes A.K.; Marder T.B.; Wade K (Editors); Royal Society of Chemistry: Cambridge, 2000, 253, 67.

POSTER PRESENTATIONS (lead author and/or presenter)

12. Sims M., Smith B., Helfrich B., Sathaye N., Messick E., Moore T., Fish R., Rajagopalan M., Rotkiewicz P., Hendricks D., Drexler K.E., and Allis D.G. "NanoEngineer-1 – A CAD-Based Molecular Modeling Program For Structural DNA Nanotechnology." Foundations of Nanoscience 2008 (FNANO08), Snowbird, UT, USA, April 22-25, 2008.

11. Allis D.G. and Korter T.M. "Understanding the Chemical Origins of Terahertz Spectra." Intelligence Community Postdoctoral Research Fellowship Colloquium, Washington, DC, USA, April 17-19, 2006.

10. Allis D.G. and Drexler K.E. "Molecular Tool Designs and Theoretical Analyses for Single Atom Mechanosynthesis." Foresight Institute 13th Conference on Molecular Nanotechnology, San Francisco, CA, USA, October 23-27, 2005.

9. Allis D.G. and Hudson B.S. "The Inelastic Neutron Scattering Spectra of Cs₂[B₁₂H₁₂] and K₂[B₁₂H₁₂]." American Chemical Society Meeting and Exposition, Washington, D.C., USA, August 28 - Sept. 1, 2005.

8. Allis D., Newlon A., Taylor J., and Spencer J.T. "New Classes of Cluster-Based High-Nonlinear Optical Response Compounds." Abstracts of Papers, 224th ACS National Meeting, Boston, MA, USA, August 18-22, 2002.

7. Allis D.G., Middleton C., Braden D., Parker S.F., and Hudson B.S. "Solid State DFT Methods and the Property Prediction of High-Symmetry Molecular Crystals." Gordon Research Conference, Vibrational Spectroscopy, Salve Regina University, Providence, RI, USA, July 28-August 2, 2002.

6. Allis D.G. and Spencer J.T. "The Use of Polyhedral Materials in Molecular Electronics and Nanostructural Applications." Foresight Institute Eighth Conference on Nanotechnology, Bethesda, MD, USA, November 3-5, 2000.

5. Allis D.G. and Spencer J.T. "New Classes of Large Nonlinear Optical Response Compounds Based Upon Polyhedral Structural Units." BUSA VII, University of Pittsburgh, Pittsburgh, PA, USA, June 7-10, 2000.

4. Allis D.G. and Spencer J.T. "The Use of Polyhedral Materials in Molecular Electronics and Nanostructural Applications." BUSA VII, University of Pittsburgh, Pittsburgh, PA, USA, June 7-10, 2000.

3. Allis D.G., Taylor J., Rudd G., and Spencer J.T. "Semiempirical and Molecular Mechanics Calculations of Polyhedral Materials in Nanostructures." Foresight Institute Seventh Conference on Nanotechnology, Santa Clara, CA, USA, October 15-17, 1999.

2. Allis D.G., Taylor J., Rudd G., and Spencer J.T. "The Use of Polyhedral Materials in Molecular Electronic and Nanostructural Applications." IMEBORON X, Durham University, Grey's College, Durham, UK, July 11-15, 1999.

1. Allis D.G., Goodisman J.S., and Spencer J.T. "Hartree-Fock and Density Functional Theoretical Considerations of the Thermal and Photochemical Pathways in Metallanonaborane Cluster Complexes." BUSA VI, The University of Georgia, Athens, GA, USA, May 14-16, 1998.

An additional, incomplete list of all presentations (including those as an associated author but non-presenter that I am aware of being on) can be found at www.somewhereville.com.

PATENTS

Pat. 2001027028 A1 20010419. Application: WO 2000-US27732 20001006. Priority: US 99-159301 19991014; US 2000-679929 20001005. Design and Fabrication of Molecular Nanostructures From Polyhedral-Based Molecular Synthetic Subunits.

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SOFTWARE

Publications with, currently using, or otherwise familiar with: Gaussian98/03, GAMESS-US and PC-GAMESS, NWChem, Crystal06, Crystal09, DMol3, CASTEP, Abinit, MPQC, MOPAC, GROMACS, NAMD, AMBER, NanoEngineer-1, associated MPI versions and numerous QC/MD GUIs (ChemOffice, CAChe, VMD, Materials Studio (Accelrys)). Unperturbed by new software (they're all just keywords and text files).

SUPPLEMENTAL INFORMATION

A more extensive CV and research description, including the ever-popular nanotechnology gallery, can be found at www.somewhereville.com.