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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, web development, science writing, science outreach.

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, Writings, Talks **Contributing Writer:** Allis D.G. "A Possible Subglacial Lake On Mars" – Free Astronomy Magazine, www.astropublishing.com, September-October 2018.

Public Lecture: Allis D.G. "The Year In Space 2018 – Things That Keep Some Of Us Up At Night" – Science Exploration Day 2018, CWS-STANYS, St. John Fisher College, Rochester, NY, May 18, 2018.

Public Lecture: Allis D.G. "Planet Nine From Outer Space" – Liverpool Public Library, Liverpool, NY, April 19, 2018.

Contributing Writer: Allis D.G. "Upstate NY Stargazing in April: The Lyrid Meteor Shower" - newyorkupstate.com, syracuse.com, April 2, 2018.

Contributing Writer: Allis D.G. "Upstate NY Stargazing in March: Two Full Moons, Venus And Mercury After Sunset" - newyorkupstate.com, syracuse.com, March 1, 2018.

Contributing Writer: Allis D.G. "Upstate NY Stargazing in February: Morning Planets And Early Notice Of A Doomed Space Station" - newyorkupstate.com, syracuse.com, February 1, 2018.

Contributing Writer: Allis D.G. "Upstate NY Stargazing in January: Supermoon, Quadrantids By Moonlight, Uranus By Binoculars" - newyorkupstate.com, syracuse.com, January 1, 2018.

Contributing Writer: Allis D.G. "Upstate NY Stargazing in December: The Geminid And Ursid Meteor Showers Close Out The Observing Year" - newyorkupstate.com, syracuse.com, November 30, 2017.

Contributing Writer: Allis D.G. "Upstate NY Stargazing in November: The Leonid Meteor Shower Takes The Stage" - newyorkupstate.com, syracuse.com, November 1, 2017.

Contributing Writer: Allis D.G. "Upstate NY Stargazing in October: The Orionids, International Observe the Moon Night" - newyorkupstate.com, syracuse.com, October 1, 2017.

Contributing Writer: Allis D.G. "Upstate NY Stargazing in September: Cassini's end and morning planet delights" - newyorkupstate.com, syracuse.com, September 1, 2017.

Contributing Writer: Allis D.G. "Stargazing in Upstate NY: What to see in the night skies August 18 to August 25" - newyorkupstate.com, syracuse.com, August 18, 2017.

Public Lecture: Allis D.G. "The Great American Eclipse (2017)" – Skaneateles Public Library, Skaneateles, NY, August 12, 2017; NOPL North Syracuse, North Syracuse, NY, August 14, 2017; Cazenovia Public Library, Cazenovia, NY, August 16, 2017; Community Library of DeWitt and Jamesville, Jamesville, NY, August 21, 2017.

Contributing Writer: Allis D.G. "Stargazing in Upstate NY: Where to find solar eclipse parties" - newyorkupstate.com, syracuse.com, August 11, 2017.

Contributing Writer: Allis D.G. "Stargazing in Upstate NY: What to see in the night skies August 4 to August 11" - newyorkupstate.com, syracuse.com, August 4, 2017.

Contributing Writer: Allis D.G. "Stargazing in Upstate NY: What to see in the night skies July 28 to August 4" - newyorkupstate.com, syracuse.com, July 28, 2017.

Contributing Writer: Allis D.G. "Stargazing in Upstate NY: What to see in the night skies July 21 to July 28" - newyorkupstate.com, syracuse.com, July 21, 2017.

Contributing Writer: Allis D.G. "Stargazing in Upstate NY: What to see in the night skies July 14 to July 21" - newyorkupstate.com, syracuse.com, July 14, 2017.

Contributing Writer: Allis D.G. "Stargazing in Upstate NY: What to see in the night skies July 7 to July 14" - newyorkupstate.com, syracuse.com, July 7, 2017.

Contributing Writer: Allis D.G. "Stargazing in Upstate NY: What to see in the night skies June 30 to July 7" - newyorkupstate.com, syracuse.com, June 30, 2017.

Contributing Writer: Allis D.G. "June Stargazing in Upstate NY: What To Look For In The Skies this Month" - newyorkupstate.com, syracuse.com, June 1, 2017.

Contributing Writer: Allis D.G. "Upstate NY Stargazing In May: A Meteor Shower And Preparations For The Solar Eclipse" - newyorkupstate.com, syracuse.com, April 31, 2017.

Contributing Writer: Allis D.G. "Upstate NY Stargazing In April: Comet Hunting And The Lyrid Meteor Shower" - newyorkupstate.com, syracuse.com, March 31, 2017.

Contributing Writer: Allis D.G. "Upstate NY Stargazing In March: Messier Marathon And The Lunar Occultation Of Aldebaran" - newyorkupstate.com, syracuse.com, March 1, 2017.

Contributing Writer: Allis D.G. "Upstate NY Stargazing In February: Lunar Eclipse, Kopernik Star Party, "Dog Nights Of Winter"" - newyorkupstate.com, syracuse.com, February 1, 2017.

Contributing Writer: Allis D.G. "Upstate NY Stargazing In January: Quadrantid Meteors And Winter's Best Early Evenings" - newyorkupstate.com, syracuse.com, January 3, 2017.

Contributing Writer: Allis D.G. "Upstate NY Stargazing In December: Geminid Meteor Shower, Another Supermoon" - newyorkupstate.com, syracuse.com, December 2, 2016.

Contributing Writer: Allis D.G. "November Stargazing In Upstate NY: Catch The Sometimes Roaring Leonids" - newyorkupstate.com, syracuse.com, October 31, 2016.

Inaugural Lecture: Allis D.G. "International Observe The Moon Night" - Technology Alliance of Central New York and Milton J. Rubenstein Museum of Science & Technology Sweet Science Series Inaugural Lecture, Syracuse, NY, October 8, 2016.

Keynote Lecture: Allis D.G. "Gravitational Waves – A New Way to Know the Universe" - Kopernik AstroFest 2016, Kopernik Astronomical Society, Vestal, NY, October 8, 2016.

Contributing Writer: Allis D.G. "Upstate NY Stargazing In October: Prominent Constellations Of summer And Winter Visible On Autumn Nights" - newyorkupstate.com, syracuse.com, October 3, 2016.

Contributing Writer: Allis D.G. "Stargazing In Upstate NY In September: Look For More Subtle Objects On Autumn Nights" - newyorkupstate.com, syracuse.com, September 6, 2016.

Contributing Writer: Allis D.G. "Stargazing In Upstate NY In August: See The Milky Way, Perseid Meteor Shower" - newyorkupstate.com, syracuse.com, August 1, 2016.

Contributing Writer: Allis D.G. "Night Sky-Gazing In Upstate NY: What To Look For In July" - newyorkupstate.com, syracuse.com, July 7, 2016.

Public Lecture: Allis D.G. "A Big Year For Dwarf Planets: Highlights Of The NASA Missions To Ceres & Pluto" - Central New York Skeptics, DeWitt, NY, January 20, 2016.

Contributing Author: Allis D.G. "Stu's Last Lesson" - Focal Point, Sky & Telescope Magazine, December, 2014

Feature Article (Cover): Allis D.G. "The 16-inch f/4.5 Collapsible-Truss Dobsonian From New Moon Telescopes: New Design Approaches and Old-Fashioned Craftsmanship" - Astronomy Technology Today, May-June 2013 (Vol. 7, Issue 3).

Invited Lecture: Allis D.G. "There's Plenty Marooned At The Bottom – The Possibilities And Politics Of Molecular Manufacturing" - SRC, Inc. Syracuse, NY January 25, 2013.

Public Lecture: Allis D.G. "A Most Unlikely Obvious Molecule – DNA And Its Consequences" - Central New York Skeptics, DeWitt, NY, November 7, 2012.

Public Lecture: Allis D.G. "Controversy In Science" - Central New York Skeptics, DeWitt, NY, January 18, 2012.

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.

Invited Lecture: Allis D.G. "I Want A New (Vitamin B₁₂-Based Bioconjugate Approach To Deliver A) Drug" and "Single Atom Manipulation And The Chemistry Of Mechanosynthesis" - 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: Allis D.G. "Single-Atom Manipulation and the Chemistry of Mechanosynthesis" - NanoScienceWorks, Taylor & Francis Publishers (www.nanoscienceworks.org/slidecast), December, 2007.

Guest Essay: Allis D.G. "Exploring the Productive Nanosystems Roadmap" - Center for Responsible Nanotechnology Newsletter (www.crnano.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

NASA Solar System Ambassador (2014-), Director of Central Intelligence Postdoctoral Research Fellow (2005-2007), Marquis Who's Who in the World, in Science and Engineering, and in America, Foresight Institute 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).

Molecular Graphics In-Print (Excluding Web Content)

Angewandte Chemie (Inside Cover, 6 June 2016), Journal of Physical Organic Chemistry (Cover, March 2014), ChemMedChem (Back Cover, April 2013), Future Medicinal Chemistry (Content, Vol. 5 No. 17, 2013), MedChemComm (Cover, September 2012), 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).

Affiliations, Organizations, Professional

International Journal of High School Research (contributing editor, 2018-), Astrofilo/Free Astronomy Magazine (contributing editor, contributing author 2018-), Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy (reviewer, 2017-), Inorganica

Activities

Chimica Acta (reviewer, 2017-), Crystal Growth and Design (Reviewer, 2017-), Astronomical League (Member-at-Large, 2016-), Ying Tri Region Science & Engineering Fair (Judge, 2013, 2014, 2015), CNY Observers & Observing (Executive Director, Lecturer 2013-), Preservation Association of Central New York (Member, Webmaster 2013-2017), Astronomy Section: Rochester Academy of Sciences (Member, 2013-), Syracuse Innovators Guild (Member, 2013-2015), Union of Concerned Scientists (Member, 2013-), Hacks/Hackers Syracuse (Member, 2012-2015), Kopernik Astronomical Society (Member, 2011-), 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), Syracuse Astronomical Society (Board of Directors, 2003-2012 and President, 2007-2012), American Association for the Advancement of Science (Member, 1997-), The Foresight Institute (Member, 1997-), The Planetary Society (Member, 1996-), American Chemical Society (Member, 1995-).

CURRENT RESEARCH AND PROFESSIONAL POSITION

Information Technology Services, Syracuse University, Syracuse, New York, USA (2015-)
Core Infrastructure Services, High Throughput and Virtual Environment Computing Support Scientist

Forensic And National Security Sciences Institute, Syracuse, New York, USA (2012-)
Research Fellow, Biological and Threat Agent Modeling and Simulation

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

Contributing Writer, Syracuse Media Group, Syracuse, New York, USA (2016-2018)
"Upstate New York Stargazing," Monthly Astronomy Writer, newyorkupstate.com and syracuse.com

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)

51. Hogg T., Moses M.S., and Allis D.G. "Evaluating the friction of rotary joints in molecular machines." *Molecular Systems Design & Engineering*, 2 (2017) 3, 235-252. DOI:10.1002/cmdc.201600073, arxiv.org/abs/1701.08202.

50. Henry K.E., Kerwood D.J., Allis D.G., Workinger J.L., Bonaccorso R.L., Holz G.G., Roth C.L., Zubieta J., and Doyle R.P. "Solution structure and constrained molecular dynamics study of vitamin B12 conjugates of the anorectic peptide PYY(3-36)." *ChemMedChem*, 11 (2016), 9, 1015-102, DOI: 10.1002/cmdc.201600073, PDB Entry: 2NA5.

49. Bonnard G., Barrès A.-L., Danten, Y., Allis D.G., Menré O., Tomerini D., Gatti C., Izgorodina E. I., Poizot P., and Frayret C. "Experimental and theoretical studies of tetramethoxy-p-benzoquinone: infrared spectra, structural and lithium insertion properties." *RSC Advances*, 3 (2013), 19081-19096, DOI: 10.1039/c3ra41974f.

48. Lashua A., Smith T., Hu H., Wei L., Allis D.G., Sponsler M., and Hudson B. "Commensurate Urea Inclusion Crystals with the Guest (E,E)-1,4-Diiodo-1,3-Butadiene." *Crystal Growth & Design*, 13 (2013), 9, 3852-3855, DOI: 10.1021/cg400980b.

47. Bonnard G., Barrès A.-L., Mentré O., Allis D.G., Gatti C., Poizot P., and Frayret C. "The low-/room-temperature forms of the lithiated salt of 3,6-dihydroxy-2,5-dimethoxy-p-benzoquinone: a combined experimental and dispersion-corrected density functional study." *CrystEngComm*, 15 (2013), 15, 2809-2821, (cover image), DOI: 10.1039/C2CE26523K.
46. Hudson B.S. and Allis D.G. "Bond alternation in infinite periodic polyacetylene: Dynamical treatment of the anharmonic potential." *Journal of Molecular Structure*, 1032 (2013) 78-82, DOI:10.1016/j.molstruc.2012.07.051.
45. Hudson B.S. and Allis D.G. "The Structure of [18]-annulene: Computed Raman Spectra, Zero-Point Level and Proton NMR Chemical Shifts." *Journal of Molecular Structure - Jaan Laane Honour Issue*, 1023 (2012) 212-215, DOI:10.1016/j.molstruc.2012.05.016.
44. Clardy-James S., Allis D.G., Fairchild T.J., and Doyle R.P. "Examining the effects of vitamin B₁₂ conjugation on the biological activity of insulin: A molecular dynamic and *in vivo* oral uptake investigation." *MedChemComm*, 3 (2012), 1054-1058, DOI:10.1039/C2MD20040F.
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.

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SUPPLEMENTAL INFORMATION

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