

**Frank Hagelberg**  
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**and Astronomy**  
**East Tennessee State University**  
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**Citizenship:** American.

**Place of Birth:** Bonn, Germany.

**Professional Positions:**

Professor of Physics at East Tennessee State University: 2013 – present

Associate Professor of Physics at East Tennessee State University: 2007 - 2013

Professor of Physics at Jackson State University: 2007

Associate Professor of Physics at Jackson State University (tenured): 2002 – 2007

Assistant Professor of Physics at Jackson State University: 1997 – 2002.

Adjunct Professor of Physics at the State University of New York at Albany: 1995 – present.

Consultant for the company “X-ray Optical Systems, Inc.” : 1994 - 1996.

Visiting Associate Professor at the State University of New York at Albany: 1992 - 1995.

Feodor Lynen Fellow at the State University of New York at Albany: 1990 - 1992.

Research and Teaching Assistant at the University of Bonn, Germany, and the Technical University of Munich, Germany, 1983 - 1990.

**Education:**

PhD in Physics: December 1989 (University of Bonn, Germany).

Diploma in Physics: January 1985 (University of Bonn, Germany).

University of Bonn, Germany, 1977 - 1978 and 1979 -1989. Studies in Physics, Physical Chemistry and Philosophy.

Gymnasium "Johanneum" of Lueneburg, Germany, 1968 - 1977

**Academic Experience:**

**(1) Teaching Activities:**

Courses taught since the Fall Semester 1991:

Undergraduate courses:

General Physics (algebra based), Technical Physics (calculus based), General and Introductory Physics Labs I and II, Quantum Mechanics, Physics of Atoms and Nuclei,

Condensed Matter Physics, Thermodynamics, Electromagnetic Theory I&II, Environmental Physics, Great Ideas of Science I&II, Technology and Human Identity (Interdisciplinary General Education Seminar).

Graduate courses:

Hyperfine Interactions as a Tool for the Study of Condensed Matter and Nuclear Systems, Mathematical Methods of Physics.

Special courses held in the framework of the “Summer Institute” of the Computational Center for Molecular Structure and Interactions, Jackson State University:

Basic Notions of Quantum Theory; The Electron Correlation Problem in Molecular Systems.

**(2) Service Activities (selected):**

Chair, Board of Directors, Institute for Computation and Research in Data Science (CaRDS): since 2018

Faculty Senator of the Department of Physics, Atmospheric Sciences, and General Science at Jackson State University, 2001 – 2004

Chair of Faculty Search Committee of the Department of Physics, Atmospheric Sciences, and General Science, 2001 - 2007.

Extensive activities in community-oriented programs at, such as organization of and participation in ‘Science Fair’ or ‘Physics Olympiad’ events directed at High School students.

Smart Node Consultant of the Cornell National Supercomputing Facility at the Albany Campus (1992 – 1996).

**Main Research Interests:**

- Theory of Atomic Cluster Systems: Analysis of growth patterns and of the origin of solid state properties (structural features, nature of bonding, ferromagnetism and antiferromagnetism, conductivity and superconductivity) by ab initio studies of finite systems,
- Spin transport through nanostructures,
- Non-adiabatic Quantum Dynamics of molecular species,
- Interactions between finite systems (molecules and clusters) with periodic substrate layers,
- Theory of electron impact excitation and ionization phenomena,
- Theory of static and dynamic Hyperfine Interactions.

**Other Professional Activities:**

Freelance writer for the science section of the German newspaper " Frankfurter Allgemeine Zeitung" (1990 – 1998)

Consulting activities related to Middle School physics curricula.

Participation in High School and Middle School Science Fairs as judge.

Reviewer for the following scientific journals: Physical Review Letters, Journal of the American Chemical Society, Physical Review (A,B), Journal of Physical Chemistry (B,C), Nuclear Instruments and Methods B, Chemical Physics Letters, Journal of Molecular Structure (Theochem), International Journal of Mass Spectrometry, International Journal of Quantum Chemistry, Journal of Molecular Modeling, Energy and Fuels, Theoretical Chemistry Accounts, Diamond and Related Materials.

Co-organizer of the AHPCRC (Army High Performance Computation Research Council) *Workshop on Verification and Validation*, Aberdeen, Maryland, October 5 – 6, 2006

**Membership in professional societies:**

American Physical Society, since 1992.

**Post-doctoral Associates:**

Dr. Chuanyun Xiao, 2/1998 – 9/2003

Dr. Sung-Soo Park, 10/2003 – 10/2004

Dr. Jianhua Wu, since 1/2004

Dr. Jian-Ge Zhou, 1/2004 – 8/2007

Dr. Dan Liu, 6/2004 – 12/2007.

**Languages:**

English, German, French.

**Awards:**

Feodor Lynen Fellow of the Alexander von Humboldt - Foundation, 1990 - 1992.

National Science Foundation Grant EPSCoR NSF-0132618. Principal Investigator. Title of research project: *Nanostructured Silicate Systems with Designed Molecular and Supermolecular Architecture*. Amount of funding: \$ 150,000. Inception of support period: 5/1/2002. Duration of support: 3 years.

Cited in the 6<sup>th</sup> Edition of "Who's who among America's Teachers", 2000.

National Science Foundation Grant CREST HRD-9805465. Principal Investigator. Title of research project: *Metal doped Silicon Clusters*. Amount of funding: \$ 863,856. Support period: 9/1/1998. 9/1/2003.

National Institute of Health /SCORE Grant S06-GM008047. Principal Investigator. Title of research project: *Novel Magnetic Resonance Imaging contrast agents from carbon nanostructures enclosing metal atom clusters*. Amount of funding: \$ 182, 840. Inception of support period: 7/1/2003: Duration of support: 2½ years.

National Science Foundation Grant CREST HRD-0318519. Principal Investigator. Title of research project: *Novel nanostructures based on low dimensional semiconductor systems*. Amount of funding: \$ 1,391,000. Inception of support period: 10/1/2003. Duration of support: 5 years.

Army High Performance Computation Research Council (AHPCRC) grant DAAD19-01-2-0014. Co-Principal Investigator. Title of research project: *Computational Studies of Biomolecules Attached to Nanoparticles*. Amount of funding: \$ 100,000/annum. Inception of support: March 2003. Duration of support: 2 years.

National Science Foundation grant DMR 0304036. Co-Principal Investigator. Title of project: *From clusters to nanoparticles: Introducing nanoscience to education and student research at Jackson State University*. Amount of funding: \$ 100,000/annum. Inception of support: June 2003. Duration of support: 1 year.

Faculty Research Productivity Award 2006, Jackson State University.

National Institute of Health/SCORE Grant S06-GM008047. Principal Investigator. Title of research project: *Multifunctional pharmaceutical agents based on carbon nanostructures with endohedral metal* Amount of funding: \$ 320,000. Inception of support period: 01/01/2006: Duration of support: 4 years.

Department of Defense Grant PE#0603755D8Z. Co-Principal Investigator. Title of project: *High Performance Computational Design of Novel Materials*. Amount of funding: \$ 120,000 per annum. Inception of support period: 10/01/2006. Duration of support: 5 years.

ETSU/RDC Grant RD0084. Principal Investigator. Title of project: *Computational studies of pharmaceuticals based on fullerenes*. Amount of funding: \$ 8,950. Inception of support period: 06/01/08. Duration of support: 1 year.

National Science Foundation (TN-SCORE, NSF EPS 1004083) First-principles studies on solar conversion processes involving nanostructured semiconductor substrates. Amount of funding: \$40,000 per annum. Inception of support period: 10/01/2010. Duration of support: 5 years.

Guest Lectureship at Innsbruck University, Innsbruck, Austria, 05/23 – 07/01/2012.

Guest Lectureship at Innsbruck University, Innsbruck, Austria, 05/06 – 06/16/2019.

#### **Invited Talks:**

*Carbon Nanostructures as media for Spin Transmission*

F.Hagelberg, Plenary Lecture, 27<sup>th</sup> Conference on Current Trends in Quantum Chemistry (CCTCC), 11/10/2018

*Nanoscale Spin Filters from Graphene Nanostructures*

Lecture, Symposium on Energy, Materials, and Nanotechnology, Vienna, Austria, 06/19/2017

*Intrinsic Magnetism in Carbon Nanostructures*

Lecture, Symposium on Energy, Materials, and Nanotechnology, Phuket, Thailand, 04/11/2016

*Magnetism in Modified Carbon Nanotubes*

Lecture, Fourth International Conference on Multifunctional, Hybrid and Nanomaterials, Sitges, Spain, 03/11/2015.

*Novel Materials Based on Carbon nanostructures*

Colloquium, Institut de Quimica Teorica i Computacional (IQTCUB), Universitat de Barcelona Barcelona, Spain, 03/09/2015.

*Computational Design of Novel Carbon Nanomaterials*

Seminar, Department of Chemistry, Jackson State University, Jackson, MS, 10/10/2014

*Computational Studies on Magnetism in Carbon Nanostructures*

Plenary lecture, 19<sup>th</sup> Symposium on Atomic and Surface Physics and Related Topics, Obergurgl, Austria, 2/16/2014

*Magnetism in Carbon Nanostructures*

Plenary lecture, 22<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/16/2013.

*Novel Materials Based on Carbon Nanostructures*

13<sup>th</sup> Southern Symposium on Computational Chemistry and Materials Science, Jackson, MS, 08/02/2013

*Novel Materials Based on Carbon Nanostructures*

Plenary lecture, 5<sup>th</sup> Conference on Methods and Applications of Computational Chemistry, Charkov, Ukraine, 07/04/2013

*Computational studies on aggregation and transport mechanisms in carbon nanostructures.*

Lecture, 2<sup>nd</sup> TN-SCORE Thrust 1 Retreat, Montgomery Bell State Park, TN, 05/21/2013

*Magnetism in single-walled carbon nanotubes of the zigzag type*

Talk, Symposium in Honor of Professor Tara Prasad Das, University at Albany, Albany, NY, 10/26/2012.

*Magnetism through Dimensional Reduction of Carbon Nanostructures*

Colloquium, Department of Chemical Engineering, Tennessee Tech University, Cookeville, TN, 03/13/2012.

*Magnetic Effects in Finite Single-Walled Carbon Nanotubes from First Principles*, Plenary lecture, Methods and Applications of Computational Chemistry, Lviv, Ukraine, 06/30/2011.

*Computational Characterization of Nanostructured Sensing Materials*. Seminar talk, delivered to DoD representatives at the Engineer Research and Development Center (ERDC), Vicksburg, MS on 08/26/2010.

*Magnetism in Novel Metallofullerenes and Ultrashort Carbon Nanotubes*, Plenary lecture, Methods and Applications of Computational Chemistry, Odessa, Ukraine, 07/02/2009.

*Magnetism in Carbon Nanostructures*, Colloquium, Appalachian State University, 04/10/09.

*Electron transfer in trimetal nitride metallofullerenes*, 6<sup>th</sup> International Conference on Computational methods in Sciences and Engineering (ICCMSE 2008), Hersonissos, Greece, 09/26/2008.

*Fullerenes enclosing trimetallic nitride clusters – the challenge of the lanthanides*, 8<sup>th</sup> Southern Symposium on Computational Chemistry and Materials Science, Jackson, MS, 04/26/2008

*Formation of Self-Assembled Monolayers on Metal and Semiconductor Substrates*, Colloquium, Department of Physics, Michigan Technological University, 10/11/2007.

*Self-assembly of thiol adsorbates on the Au(111) surface*  
Lester Symposium, University of California at Berkeley, 03/31/2007

*Computational studies on cage-like clusters*  
Department of Physics, Northeastern Illinois University, 03/23/2006

*Cage-like clusters with endohedral metal impurities*  
Department of Physics, East Tennessee State University, 02/28/2006

*Computational studies on endohedral and deposited silicon based clusters*  
Department of Chemistry, Texas Tech University, 01/25/2006.

*Cage-like clusters enclosing atomic and molecular impurities*  
Department of Physics, Mississippi State University, 10/3/2005.

*Free and deposited silicon based clusters: a computational study*  
Department of Physics, University of New Hampshire, 4/21/2005.

*Carbon and silicon cage clusters with endohedral impurities*  
International Electron Ion Symposium, Igls, Austria, May 2004.

*Molecular cages encapsulating metal cluster impurities*  
Department of Chemistry, Mississippi State University, 1/23/2004

*Silicon clusters with endohedral metal atom impurities*  
Department of Chemistry, Johns Hopkins University, 1/15/2004

*Nonadiabatic Evolution of Electronic States by Electron Nuclear Dynamics Theory*  
Third Southern School of Computational Chemistry, Orange Beach, AL, March 2003.

*The Mathematics of Many Particles*  
Seminar talk, held in the Mathematics Department of Jackson State University.,  
4/25/2002.

*The Hybrid World of Atomic Clusters*  
Seminar talk, held at Jackson State University in the frame of the program "Research Thursday", designated to highlight outstanding achievements of JSU researchers,  
3/28/2002.

*Cage-like Silicon Clusters with Endohedral Metal Atom Impurities*  
Second Southern School of Computational Chemistry, Orange Beach, AL, March 2002.

*Pseudorotational Dynamics of Small Molecular Species*  
XIIIth Symposium on Atomic and Surface Physics and Related Topics, Going, Austria,  
2/22/2002

*Non-adiabatic Effects in the Pseudorotational Motion of Triatoms*  
Seminar talk, University of Florida, 08/23/2001.

*Silicon Clusters with Metal Atom Impurities*  
Seminar talk, University of Innsbruck, Austria, 07/5/2001.

*Silicon Clusters with Metal Atom Impurities*  
Northeastern Regional Meeting of the American Chemical Society, Durham, NH, June  
2001.

*Pseudorotational Dynamics of Triatomic Systems*  
Second Southern Symposium on Computing, Hattiesburg, MS, 10/23/2000.

*Theoretical Investigations on pure and doped Silicon Clusters*  
University of Mississippi, Colloquium, Department of Physics, 9/26/2000.

*Theoretical Investigations on Silicon Clusters*  
University of Hawaii at Manoa, Colloquium, Department of Physics, 4/6/2000.

*Electron Nuclear Dynamics of Small Molecular Systems*  
University of California at Berkeley, 10/22/1999.

*Electron Nuclear Dynamics of Small Molecular Systems*  
First Southern Symposium on Computing, Hattiesburg, MS, December 1998.

*Quantum Dynamics of Small Molecular Systems*  
University of Southern Mississippi, 11/20/1998.

*Electron Nuclear Dynamics Studies of Triatomic Systems*  
Central Michigan University, 11/5/1998.

*Stabilization Mechanisms for Zintl Clusters*  
Conference on Physics of Clusters - Clusters in Plasma and Gases, Pushchino, Moscow Region, Russia, August 1997.

*Antimony Based Zintl Clusters*  
Jackson State University, 12/5/1996.

*Geometric Phases in Near - Degenerate Systems*  
Conference on Quantum Mechanics from Microcosm to Macrocosm, Albany, NY, April 1996.

*Theoretical Investigations on Zintl Clusters*  
University of Cincinnati, 11/20/1995.

*Ab Initio Investigations on Sb<sub>4</sub> based Clusters*  
The Pennsylvania State University, 11/4/1994.

*The Origin of Transient Magnetic Fields*  
Marshall University, 04/22/1994.

*Ab Initio Investigations on Alkali-Antimony Systems*  
University of Konstanz, Germany, 01/14/1994.

*Ab Initio Investigations on Alkali-Antimony Systems*  
University of Erlangen, Germany, 01/12/1994.

*On the Origin of Transient Magnetic Fields*  
Symposium on Local Order in Condensed Matter Physics, Jekyll Island, GA, June 1993.

*Transient Magnetic Fields*  
College of New Paltz, 12/10/1991.

*Transient Magnetic Fields*  
Rutgers University. 09/12/1991.

*The Physics of Transient Fields*  
SUNY at Albany, 10/6/1990,

**Regular contributions to national and international conferences since 1997:**

(114) Spin transport properties of  $z\text{CrX}_2$  ( $X = \text{S}, \text{Se}$ ) nanoribbons  
F.Hagelberg, Poster, 61<sup>th</sup> Sanibel Symposium, 2/15/2022

(113) Spin-dependent Transport in Transition Metal Dichalcogenide Nanoribbons  
F.Hagelberg, Poster/Talk, 2021 eSSSENCE meeting on "Multiscale modelling of materials and molecules", Uppsala, Sweden, 6/7/2021



- (112) Spin-dependent Transport in Transition Metal Dichalcogenide Nanoribbons  
F.Hagelberg, Poster/Talk, 2020 eSSSENCE meeting on "Multiscale modelling of materials and molecules", Uppsala, Sweden, 6/8/2020
- (111) Spin Transport Properties of Armchair Graphene Nanoribbons with Substitutional Transition Metal atoms  
F.Hagelberg, Poster, 60<sup>th</sup> Sanibel Symposium, 2/18/2020
- (110) Transition Metal Dichalcogenide Monolayers as Media for Spin Transport  
F.Hagelberg, Poster, 28th Conference on Current Trends in Quantum Chemistry (CCTCC), 11/13/2019
- (109) Giant Magnetoresistance in Transition Metal Dichalcogenide Monolayers  
F.Hagelberg, Poster, 59<sup>th</sup> Sanibel Symposium, 2/18/2019
- (108) Half-metallicity in strained graphene nanoribbon devices with vacancies  
F.Hagelberg, Talk, 58<sup>th</sup> Sanibel Symposium, 2/21/2018
- (107) Strained zigzag graphene nanoribbon devices with vacancies as perfect spin filters  
M.Magno, F.Hagelberg, Poster, 26<sup>th</sup> Conference on Current Trends in Quantum Chemistry (CCTCC), 11/10/2017
- (106) Spin filter properties of armchair graphene nanoribbons with substitutional Fe atoms  
F. Hagelberg, A.Kaiser, I.Sukuba, M. Probst, Poster, 57<sup>th</sup> Sanibel Symposium, 2/21/2017
- (105) Designing a spin filter circuit based on a finite single-walled carbon nanotube of the zigzag type  
O.V. Khavryuchenko, G.H. Peslherbe, F.Hagelberg, Poster, 25th Conference on Current Trends in Quantum Chemistry (CCTCC), 11/13/2016.
- (104) Spin dependent electron transmission through single-walled carbon nanotubes of the zigzag type  
O.V. Khavryuchenko, G.H. Peslherbe, F.Hagelberg, Poster, 56<sup>th</sup> Sanibel Symposium, 2/16/2016
- (103) Vacancies promise a possible route towards artificial patterning of self-assembled monolayers  
A.Kaiser, F.Vines, F.Illas, M.Ritter, F.Hagelberg, M.Probst, Poster, Fourth International Conference on Multifunctional, Hybrid and Nanomaterials, Sitges, Spain, 03/10/2015.
- (102) A spin filter circuit design based on a finite single-walled carbon nanotube of the zigzag type  
O.Khavryuchenko, G.Peslherbe, F. Hagelberg, Poster, 54th Sanibel Symposium, Saint Simon Island, GA, 02/16/2015

(101) Cross-Linking Carbon Nanotubes: Geometric, Magnetic, and Adsorption Properties.

J.Wu, A. Ayasoufi, J. Leszczynski, F. Hagelberg, Poster, 53<sup>th</sup> Sanibel Symposium, Saint Simon Island, GA, 02/18/2013

(100) Metal Dihydrides Encapsulated in Polyhedral Oligomeric Silsesquioxane Cages of the T8 and T10 types.

Xiqiao Wang, Alyssa Spooner, John Corn, Frank Hagelberg, Poster, 21<sup>st</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/03/2012

(99) Polyhedral Oligomeric Silsesquioxane Cages with Endohedral Metal Hydrides.

Xiqiao Wang, Alyssa Spooner, John Corn, Frank Hagelberg, Poster, TN-SCORE Annual conference, Nashville, TN 06/15/2012

(98) Hydrogen Storage in Polyhedral Oligomeric Silsesquioxane Cages.

Alyssa Spooner, Frank Hagelberg, Poster, TN-SCORE, Thrust-1 Retreat, Montgomery Bell State Park, TN 04/27/2012

(97) Do Stone-Wales defects alter the magnetic and transport properties of single-walled carbon nanotubes?

Frank Hagelberg, Poster, 52<sup>th</sup> Sanibel Symposium, Saint Simon Island, GA, 02/20/2012

(96) Cross-linking carbon nanotube architectures with adsorbed H-atoms: structural and magnetic features, Jianhua Wu, Frank Hagelberg, Poster, 20<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 10/29/2011

(95) Ferrocyanide-alkali complexes as electrolytes in photoelectrochemical solar cells, Alyssa Spooner, Frank Hagelberg, Poster, TN-SCORE Annual Conference, Nashville, TN 08/08/2011.

(94) Do Stone-Wales defects alter the magnetic and transport properties of single-walled carbon nanotubes? J. Wu, Tandabany C. Dinadayalane<sup>c</sup>, Danuta Leszczynska, Jerzy Leszczynski, F. Hagelberg. Poster, 11<sup>th</sup> Southern School on Computational Chemistry and Materials Science. Jackson, MS, 07/28 /2011.

(93) Magnetic moments of zigzag single-walled carbon nanotubes:dependence on curvature and topological defects, F.Hagelberg, Poster, 51<sup>th</sup> Sanibel Symposium, Saint Simon Island, GA, 02/27/2011.

(92) Theoretical study on the insertion of atomic lanthanide impurities into single walled carbon nanotubes of the zigzag type. F. Hagelberg, J.Wu; Poster, 19<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 10/29/2010.

(91) Computational studies on the diameter dependence of magnetic moments of zigzag single wall carbon nanotubes. J. Wu, F. Hagelberg; Poster, 19<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 10/29/2010.

(90) First principle calculations on the electronic and magnetic properties of zigzag single wall carbon nanotubes with Stone-Wales defects. J. Wu, F. Hagelberg , T.C.

Dinadayalane, J.Leszczynski; Poster, 19<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 10/30/2010.

(89) Magnetic moments of finite single walled carbon nanotubes: variation with tube size. Poster, J. Wu, F.Hagelberg; Poster, 10<sup>th</sup> Southern School on Computational Chemistry and Materials Science. Jackson, MS; 04/24/2010.

(88) Hydrocarbon Adsorbates on Single Walled Carbon Nanotubes of Finite Length. Poster, F. Hagelberg, J. Wu, 50<sup>th</sup> Sanibel Symposium, Saint Simon Island, GA, 02/28/2010.

(87) Computational studies on the adsorption of small hydrocarbon radicals on finite single wall carbon nanotubes. Poster, J. Wu, F. Hagelberg, 18<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 10/31/2009.

(86) Hydrogen Storage in Polyhedral Oligomeric Silsesquioxanes by Encapsulating Metal Hydrides. Poster, J.Corn, B.Bailey, F. Hagelberg, 18<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 10/30/2009.

(85) Magnetic Fullerenes and Carbon Nanotubes. Talk, F.Hagelberg, 9<sup>th</sup> Southern School on Materials Science and Computational Chemistry, Jackson, MS, 07/28/2009.

(84) Mechanism for inserting Gd atoms into finite single wall carbon nanotubes of the zigzag type. Poster, J. Wu, F.Hagelberg, 9<sup>th</sup> Southern School on Materials Science and Computational Chemistry, Jackson, MS, 07/28/2009.

(83) Computational study on cross-linking single wall carbon nanotube architectures. Poster, J. Wu, F.Hagelberg, 9<sup>th</sup> Southern School on Materials Science and Computational Chemistry, Jackson, MS, 07/28/2009.

(82) Magnetism in Finite-Size Single Walled Carbon Nanotubes of the Zigzag Type. Poster, F.Hagelberg, St. Simons Island, GA, 03/01/2009.

(81) Self-Assembly of Methanethiol Adsorbates on Metal Surfaces. Talk, F. Hagelberg, Zing conference on nanomaterials, Playa del Carmen, Mexico, 12/8/2008.

(80) The role of metal substrate reconstruction in the self-assembly of thiol adsorbates. Poster, Frank Hagelberg, Georgi Nenchev, Bogdan Diaconescu, Karsten Pohl, 17<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/02/08.

(79) Theoretical Study on the Magnetism in Finite Size Single Wall Carbon Nanotubes. Poster, Jianhua Wu, Frank Hagelberg, 17<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/02/08.

(78) Adsorption of CH<sub>2</sub> and CH<sub>3</sub> on a single walled carbon nanotube of the (10,0) type. Poster, Jianhua Wu, Frank Hagelberg, 8<sup>th</sup> Southern Symposium of Computational Chemistry and Materials Science, Jackson, MS, 04/26/2008.

(77) Dimerization of Methanethiol Adsorbates on Metal Surfaces. Poster, Frank Hagelberg, 47<sup>th</sup> Sanibel Symposium, St.Simons Island, GA, 02/23/2007

- (76) Chemistry in Acetone Complexes of Metal Dications: A Remarkable Ethylene Production Pathway. Poster, Frank Hagelberg, Jianhua Wu, , Sung Soo Park, Alexandre A. Shvartsburg, 16<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/02/07.
- (75) Investigation of optical polymers with improved chemical properties. Poster, Sung Soo Park, Frank Hagelberg, 16<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/03/07.
- (74) Intermolecular Electron Transfer in Dimetallofullerenes Based on C<sub>84</sub> and C<sub>86</sub>. Poster, Dan Liu, Frank Hagelberg, 16<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/02/07.
- (73) Investigation of optical polymers with improved chemical properties. Poster, Sung Soo Park, Frank Hagelberg, 16<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/03/07.
- (72) Impact of internal electron transfer on the structure of C74 encapsulating Sc and La metal atom impurities. Poster, D.Liu, F.Hagelberg, 7<sup>th</sup> Southern School of Quantum Chemistry and Materials Science, Jackson, MS, 04/06/07.
- (71) First Principles Calculations on Three-Dimensional Silicon Clusters Adsorbed on Graphite (0001) and Diamond (100) Substrates. Poster, presented at the 7<sup>th</sup> Southern School of Quantum Chemistry and Materials Science; J.Wu, F.Hagelberg, Jackson, MS, 04/07/07.
- (70) Self-Assembly of Thiols on the Au(111) surface: Dimerization. Talk, presented at the 7<sup>th</sup> Southern School of Quantum Chemistry and Materials Science; J.G.Zhou, Q.Williams, F.Hagelberg, Jackson, MS, 04/06/07.
- (69) Dimerization of thiol adsorbates on the Au(111) surface. Talk, Frank Hagelberg, March Meeting of the American Physical Society 2007, Denver, CO, 03/06/2007.
- (68) Cage-core interactions in fullerenes enclosing metal clusters with multiple scandium and yttrium atoms; Dan Liu, Frank Hagelberg. Talk, presented at the March Meeting of the American Physical Society 2007, Denver, CO, 03/05/2007.
- (67) Chemisorption of alkanethiol molecules on the Au(111) surface. Frank Hagelberg, Jian-Ge Zhou. Poster, presented at the 47<sup>th</sup> Sanibel Symposium, St.Simons Island, GA, 03/23/2007.
- (66) Self-assembly of thiol adsorbates on the Au(111) surface. Frank Hagelberg, Jian-Ge Zhou. Poster, presented at the Advanced workshop on nanomaterials, Trieste, Italy 01/22/2007.
- (65) Extending the Hueckel 4n+2 Rule to Metallofullerenes: The Example of M<sub>2</sub>@C<sub>84</sub> (M=Sc, Y); Dan Liu, Frank Hagelberg. Poster, presented at the 15<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/04/06.

(64) Do Methanethiol Adsorbates on the Au(111) Surface Dissociate? J.G.Zhou, Frank Hagelberg. Poster, presented at the 15<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/04/06.

(63) Ethylene Production in the Collision Induced Dissociation of Metal Dication-Acetone<sub>n</sub> Complexes. Jianhua Wu, Frank Hagelberg, Alexandre A. Shvartsburg. Poster, presented at the 15<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/03/06.

(62) Cage-Core Interactions in Fullerenes Enclosing Metal Clusters with Multiple Scandium Atoms. Sung Soo Park, Dan Liu, Frank Hagelberg. Poster, presented at the XII. International Congress in Quantum Chemistry, Kyoto, Japan, 05/23/2006.

(61) Adsorption behavior of methanethiol molecules on the Au(111) surface dissociate? Jian-Ge Zhou, F.Hagelberg, Talk, presented at the 6<sup>th</sup> Southern School on Computational Chemistry, Jackson, MS, 04/07/2006.

(60) Comparative investigation of three dimensional Si clusters on graphite and diamond substrates, Jianhua Wu, F.Hagelberg, Poster, presented at the 6<sup>th</sup> Southern School on Computational Chemistry, Jackson, MS, 04/07/2006.

(59) Understanding the unique architecture of Sc<sub>x</sub>@C<sub>82</sub> (x=1, 2 and 3) by use of the 4n+2 rule.  
Dan Liu, F.Hagelberg. Poster, presented at the 6<sup>th</sup> Southern School on Computational Chemistry, Jackson, MS, 4/7/2006.

(58) Geometric and electronic structure of mixed metal-semiconductor clusters from global optimization.  
J.H. Wu, F.Hagelberg. Talk, presented at the March Meeting of the American Physical Society 2006, Baltimore, MD, 3/14/2006.

(57) Coverage dependence of 1-propanol adsorption on the Si(001) surface and fragmentation dynamics.  
J.H. Wu, F.Hagelberg. Talk, presented at the March Meeting of the American Physical Society 2006, Baltimore, MD, 3/14/2006.

(56) Fragmentation dynamics of 1-propanol molecules deposited on the Si(001) surface.  
Frank Hagelberg. Poster, presented at the 46<sup>th</sup> Sanibel Symposium, St.Simons Island, GA, 3/2/2006.

(55) Relationship between structural stability and cage-core interaction for Sc<sub>3</sub>@C<sub>82</sub> and Sc<sub>2</sub>@C<sub>84</sub>.  
Dan Liu, Frank Hagelberg. Poster, presented at the 14<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/04/05.

(54) Equilibrium geometries of mixed metal-semiconductor clusters from global optimization and associated electronic properties.  
Jianhua Wu, Frank Hagelberg. Poster, presented at the 14<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/05/05.

- (53) Chemisorption of alkanethiols on Au(111): Is it dissociative or non-dissociative?  
Jian-Ge Zhou, Frank Hagelberg. Poster, presented at the 14<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/05/05.
- (52) Fragmentation dynamics of organic species deposited on a semiconductor substrate.  
Frank Hagelberg, Jian-Ge Zhou. Poster, presented at the 14<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/05/05.
- (51) Computational study on the coverage dependence of 1-Propanol molecules on the Si(100) Surface.  
Jian-Ge Zhou, Frank Hagelberg. Poster, presented at the 5<sup>th</sup> Southern School on Computational Chemistry, Jackson, MS, 4/8/2005.
- (50) Interaction of small deposited silicon clusters with graphite surfaces.  
Jianhua Wu, Jian-Ge Zhou, Frank Hagelberg. Poster, presented at the 5<sup>th</sup> Southern School on Computational Chemistry, Jackson, MS, 4/8/2005.
- (49) Endohedral silicon clusters containing atomic and ionic impurities.  
Delwar Hossain, C.U.Pittman, Svein Saebo, Frank Hagelberg. Talk, presented at the 5<sup>th</sup> Southern School on Computational Chemistry, Jackson, MS, 4/8/2005.
- (48) An orbital physics study on coexisting electron transfer and hybridization mechanisms in NSc<sub>3</sub> metallofullerenes.  
Dan Liu, Frank Hagelberg. Talk, presented at the 5<sup>th</sup> Southern School on Computational Chemistry, Jackson, MS, 4/8/2005.
- (47) Cage structures based on Polyhedral Oligomeric Silsesquioxanes (POSS) with atomic and ionic impurities.  
Frank Hagelberg, Sung Soo Park, Chuanyun Xiao, Delwar Hossein, Charles Pittman, Svein Saebo. Talk, presented at the March Meeting of the American Physical Society 2005, Los Angeles, CA, 3/23/2005.
- (46) Computational studies on small silicon clusters deposited on a graphite substrate.  
Frank Hagelberg and Jianhua Wu, Talk, presented at the March Meeting of the American Physical Society 2005, Los Angeles, CA, 3/23/2005.
- (45) Analysis of non-adiabatic phenomena in ion-atom and ion-molecule interactions,  
Frank Hagelberg.  
Poster, presented at the 45<sup>th</sup> Sanibel Symposium, St.Simons Island, GA, 3/7/2005.
- (44) Molecular Orbital Theory of the Mechanism Underlying the Haldane Gap in Spin-1/2 NaTiSi<sub>2</sub>O<sub>6</sub> and the Spin-Peierls Transition in Spin-1 LiVGe<sub>2</sub>O<sub>6</sub>.  
Dan Liu and Frank Hagelberg. Poster, presented at the 13<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/13/04.
- (43) "Polyhedral Oligomeric Silsesquioxanes (POSS) Cages with Alkali, Noble Gas and Halogen Impurities".

Delwar Hossain, Charles U. Pittman, Jr., Svein Saebo, Sung Soo Park, Chuanyun Xiao, and Frank Hagelberg. Poster, presented at the 13<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/13/04.

(42) "Computational Investigations of Small Silicon Clusters on a Graphite Substrate"  
Jianhua Wu, Jian-Ge Zhou, and Frank Hagelberg. Poster, presented at the 13<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/13/04.

(41) "Adsorption of 1-Propanol on the Si(100) Surface"  
Jian-Ge Zhou, and Frank Hagelberg. Poster, presented at the 13<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/12/04.

(40) "Nonadiabatic Evolution of Electronic States by Electron Nuclear Dynamics Theory: Application to Atom-Molecule Scattering Problems".  
Talk, presented at the March Meeting of the American Physical Society 2004, Montreal, CA, 3/25/2004.

(39) "Non-classical Fullerene Cages Enclosing Metal Atom Clusters".  
Talk, presented at the March Meeting of the American Physical Society 2004, Montreal, CA, 3/24/2004.

(38) "Nonadiabatic Effects in Atom-Molecule Scattering by Electron Nuclear Dynamics Theory."  
Poster, presented at the 44<sup>th</sup> Sanibel Symposium, St. Augustine, FL, 3/2/2004.

(37) "Substitutional and Endohedral Structures Based on Polyhedral Oligomeric Silsesquioxane (POSS) Molecules"  
C. Xiao, F. Hagelberg. Poster, presented at the 12<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/2/03.

(36) "Structures and Dissociation Channels of Metal Dications Solvated by Acetonitrile Ligands"  
F. Hagelberg, C.Xiao, A. El-Nahas. Poster, presented at the 12<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/2/03.

(35) "Determination of the nonadiabatic content of dynamic molecular systems by Electron Nuclear Dynamics Theory"  
F. Hagelberg. Poster, presented at the 12<sup>th</sup> International Conference on Quantum Chemistry, Bonn, Germany, 7/25/03.

(34) "Interaction of 3d transition metal atoms with charged projectiles from Electron Nuclear Dynamics computation"  
Talk, presented at the March Meeting of the American Physical Society 2003, Austin, TX, 3/3/2003.

(33) "Computational study on multiply charged metal ions ligated with DMSO".  
Talk, presented at the March Meeting of the American Physical Society 2003, Austin, TX, 3/3/2003.

- (32) "Interaction of 3d transition metal atoms with ion projectiles from Electron Nuclear Dynamics computation"  
Poster, presented at the 43<sup>rd</sup> Sanibel Symposium, St. Augustine, FL, 2/25/2003.
- (31) "The Decay of Metastable Ne<sub>2</sub><sup>+</sup>: Experiment and Theory."  
Poster, presented at the 11<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/2/02.
- (30) "Comparative Study of Small Silicon Clusters with Cu, Sc and Y Dopants"  
J.Blundell, C.Xiao, F.Hagelberg. Poster, presented at the 11<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/1/02.
- (29) "Electron Nuclear Dynamics of Vibronic Interactions in Small Molecules"  
F.Hagelberg. Poster, presented at the "International Conference on Theoretical Physics (TH2002)",  
Paris, France, 7/25/02.
- (28) "Non-adiabatic effects in the pseudorotational motion of triatomic molecules"  
F.Hagelberg. Talk, presented at the "March Meeting of the American Physical Society 2002", Indianapolis, IN, 3/21/02.
- (27) "Geometric and electronic structure of MeSi(n) (Me = Mo, W; n = 1 – 6, 12)"  
F.Hagelberg. Talk, presented at the "March Meeting of the American Physical Society 2002", Indianapolis, IN, 3/18/02.
- (26) "Small Silicon Clusters with 3d Transition Metal Atom Impurities"  
A.Abraham, R.Quinn, C.Xiao, F.Hagelberg, I.Ovcharenko, W.A.Lester, Jr. Poster, presented at the 10<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/1/01.
- (25) "Cage-like Clusters of composition MeSi<sub>12</sub> with Me=Cr, Mo, W"  
C.Xiao, F.Hagelberg, I.Ovcharenko, W.A.Lester Jr. Poster, presented at the 10<sup>th</sup> Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/3/01.
- (24) "Ionization energies of rare gas and molecular clusters determined by high resolution electron impact"  
P.Scheier, M.Ruemmele, T.Fiegele, G.Hanel, B.Gstir, M.Stano, A.Stamatovic, F.Hagelberg, T.D.Maerk.  
Invited Talk, presented by P.S. at the International Symposium on Electron – Molecule Collisions and Swarms, Lincoln, NE, 7/15/01.
- (23) "Geometric and electronic features of Copper doped Silicon Clusters."  
F.Hagelberg.  
Talk, presented at the March Meeting 2001 of the American Physical Society (APS), Seattle,WA, 3/16/01.
- (22) "Pseudorotational Dynamics of Small Molecular Species."  
F.Hagelberg,  
Talk, presented at the March Meeting 2001 of the American Physical Society (APS), Seattle,WA, 3/15/01.



(21) "Pseudorotational Dynamics of Triatomic Systems – Extension to the Non-Adiabatic Regime."

F.Hagelberg.

Poster, presented at the "41<sup>th</sup> Sanibel Symposium", St.Augustine, FL, 2/27/01.

(20) "A Density Functional Investigation of MoSi<sub>N</sub> (N=1 – 6) Clusters."

J.G.Han, F.Hagelberg.

Poster, presented at the 9<sup>th</sup> conference "Current Trends in Computational Chemistry" at Vicksburg, MS, 11/5/00.

(19) "Copper-Silicon Interaction in CuSi<sub>N</sub> (N= 4 – 12) Clusters"

C.Xiao, F.Hagelberg.

Poster, presented at the 9<sup>th</sup> conference "Current Trends in Computational Chemistry" at Vicksburg, MS, 11/4/00.

(18) "Cocaine Abuse Treatment Agents: Theoretical Study of Methylphenidate Analogues Using *Ab Initio* and Semi-Empirical Molecular Orbital Calculations."

B.Ojo, F.Hagelberg, C.Xiao, L.Kincaid, J.Leszczynski.

Poster, presented at the 9<sup>th</sup> conference "Current Trends in Computational Chemistry" at Vicksburg, MS, 11/4/00.

(17) "Theoretical Investigation on Small Silicon and Carbon Clusters Deposited on a Graphite Layer."

F.Hagelberg, P.Scheier, K.Sattler, B.Marsen, M.Lonfat.

Poster, presented at the "10<sup>th</sup> International Symposium on Small Particles and Inorganic Clusters" at Atlanta, GA, 10/12/00.

(16) "Quasi-spherical Structures of Copper-doped Silicon Clusters (CuSi<sub>N</sub>, N < 13)."

C.Xiao, F.Hagelberg.

Poster, presented at the "4<sup>th</sup> Canadian Computational Chemistry Conference" at Lennoxville, Canada, 8/1/00.

(15) "Pseudoprecession of threeatomic cations by Electron Nuclear Dynamics Theory."

F.Hagelberg.

Poster, presented at the "International Congress on Quantum Chemistry" Mentone, France, 6/4/00.

(14) "Coriolis Coupling in Threeatomic Molecular Species."

F.Hagelberg.

Poster, presented at the "40<sup>th</sup> Sanibel Symposium", St.Augustine, FL, 2/28/99.

(13) "Coulomb Blockade effects in Charged Si<sub>7</sub> Clusters on Graphite Substrate".

F.Hagelberg.

Poster, presented at the 8<sup>th</sup> conference "Current Trends in Computational Chemistry" at Vicksburg, MS, 11/6/99.

(12) "Spin Transfer as Stabilization Mechanism for O<sub>2</sub> and O<sub>3</sub> Analogous Zintl Clusters".

D.Spencer, F.Hagelberg.

Poster, presented at the 8<sup>th</sup> conference “Current Trends in Computational Chemistry” at Vicksburg, MS, 11/6/99.

(11) “Surface States of Cu impurities in Small Copper – Silicon clusters”.

C.Xiao, F.Hagelberg.

Poster, presented at the 8<sup>th</sup> conference “Current Trends in Computational Chemistry” at Vicksburg, MS, 11/6/99.

(10) “Computational studies on Si<sub>7</sub> clusters deposited on a graphite substrate”.

F.Hagelberg, P.Scheier, B.Marsen, M.Lonfat, K.Sattler.

Poster, presented at the conference “International Symposium of Clusters and Interfaces”, Richmond, October 99.

(9) “Electron Nuclear Dynamics Investigations of three – and fouratomic molecules.”

F.Hagelberg.

Talk, given at the “APS Centennial Meeting”, Atlanta, GA, 3/24/99.

(8) “Quantum Dynamical Investigations on H<sub>3</sub> and Li<sub>3</sub>.”

F.Hagelberg.

Poster, presented at the “Thirty – Ninth Sanibel Symposium”, St.Augustine, FL, 3/1/99.

(7) “Quantum Dynamical Computations on the Li<sub>3</sub> Molecule using the END Theory.”

F.Hagelberg, E.Deumens, Y.Oehrn.

Poster, presented at the 7<sup>th</sup> conference “Current Trends in Computational Chemistry” at Vicksburg, MS, 11/6/98.

(6) “Theoretical Investigations on Cage-like Silicon Clusters Doped with Cu Atoms.”

F.Hagelberg, I.Yanov, J.Leszczynski.

Poster, presented at the 7<sup>th</sup> conference “Current Trends in Computational Chemistry” at Vicksburg, MS, 11/6/98.

(5) “O<sub>2</sub> and O<sub>3</sub> analogous clusters based on groupVA elements.”

Daryl Spencer, F.Hagelberg.

Poster, presented at the 7<sup>th</sup> conference “Current Trends in Computational Chemistry” at Vicksburg, MS, 11/6/98.

(4) “Theoretical Investigations on Closed-Shell Silicon<sub>N</sub> Clusters with N ≤ 26.”

F.Hagelberg, J.Leszczynski, V.Murashov.

Poster, presented at the International Symposium for Particles and Inorganic Clusters (ISSPIC9) at Lausanne, Switzerland, 9/2/98.

(3) “Quadrupole Moment of the Mossbauer Active 57mFe Nucleus”

F.Hagelberg, T.P.Das, K.C.Mishra.

Talk, given at the March Meeting 1998 of the American Physical Society, Los Angeles, CA, 3/20/98.

(2) “Theoretical Investigations on Closed-Shell Silicon<sub>N</sub> Clusters with N ≤ 26”

F.Hagelberg, J.Leszczynski, A.Korkin, V.Murashov.

Poster, presented at the 6<sup>th</sup> conference “Current Trends in Computational Chemistry”, 11/7/97.

(1) "Evaluation of the  $^{57}\text{Fe}$  quadrupole moment from Hartree-Fock Investigations"  
F.Hagelberg, T.P.Das.  
Poster, presented at the XIVth International Symposium on Nuclear Quadrupole Interactions, Pisa, Italy, 7/21/97.

### References:

1. Prof. Y.Öhrn, Quantum Theory Project, University of Florida, Gainesville, FL 32611.  
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## Publications

### Books

- F.Hagelberg, *Electron Dynamics in Molecular Interactions*, Imperial College Press, London (2014)
- F.Hagelberg, *Magnetism in Carbon Nanostructures*, Cambridge University Press (2017)
- F.Hagelberg, T.Dinadayalane (eds.), *Properties and Functionalization of Graphene*, Elsevier (2022)

## Refereed research articles

(117) Spin Transport Properties of zCrXY (X, Y = S,Se) Nanoribbons: Implications for Spintronics

R. Yeatts, F.Hagelberg, J. Phys. Chem. C 2022, 126, 42, 18115 (2022)

(116) Toward graphene-based devices for nanospintronics

M.Magno, F.Hagelberg, in: Properties and Functionalization of Graphene, Elsevier (2022)

(115) Half-Metallic Devices from Armchair Graphene Nanoribbons with Transition Metal Guest Atoms

F.Hagelberg, J.R.Romero, M.Probst, O. Khavryuchenko, Chem.Select 6, 347 (2021)

(114) Highly Stable [C<sub>60</sub>AuC<sub>60</sub>]<sup>+/-</sup> Dumbbells

M. Goulart, M. Kuhn, P.Martini, L. Chen, F. Hagelberg, A. Kaiser, P.Scheier, A. M. Ellis, J.Phys.Chem.Lett. 9, 2703 (2018)

(113) Strained zigzag graphene nanoribbon devices with vacancies as perfect spin filters

M. Magno, F. Hagelberg, The Journal of Molecular Modeling, 24(1) (2018)

(112) Spin filter properties of armchair graphene nanoribbons with substitutional Fe atoms

F. Hagelberg, A.Kaiser, I.Sukuba, M. Probst, Mol. Phys. 115, 2231 (2017)

(111) Spin Filter Circuit Design Based on a Finite Single-Walled Carbon Nanotube of the Zigzag Type

O.V. Khavryuchenko, G. H. Peslherbe, F. Hagelberg, J. Phys. Chem. C 119, 3740 (2015).

(110) Vacancy patterning and patterning vacancies: controlled self-assembly of fullerenes on metal surfaces

A.Kaiser, F. Vines, F. Illas, M. Ritter, F.Hagelberg, M.Probst, Nanoscale 6, 10850 (2014).

(109) Intrinsic Magnetism in Single-Walled Carbon Nanotubes of Finite Length

F. Hagelberg, J. Wu, A. Ayasoufi, J. Leszczynski, in: Practical Aspects of Quantum Chemistry III, ed. J. Leszczynski, M.Shukla, Springer, New York, 2014.

(108) Aggregates of PCBM molecules: A computational study.

A. Kaiser, M.Probst, H. A. Stretz, F. Hagelberg, Int. Jour.Mass Spec. 325, 225 (2014).

(107) Ordered phases of ethylene adsorbed on charged fullerenes and their aggregates, S.Zoettl, A.Kaiser, M.Daxner, M.Goulart, A.Mauracher, M.Probst, F.Hagelberg, S.Denifl, P.Scheier, O.Echt, Carbon 69, 206 (2014).

(106) Endohedral Complexes of Polyhedral Oligomeric Silsesquioxane (POSS) cages

- with Transition Metal Dihydrides, X. Wang, F.Hagelberg, Chem.Phys. 426, 48 (2013).
- (105) Impact of Tube Curvature on the Ground-State Magnetism of Axially Confined Single-Walled Carbon Nanotubes of the Zigzag Type, J. Wu, F.Hagelberg, ChemPhysChem 14, 1696 (2013)
- (104) Geometric, Magnetic, and Adsorption Properties of Cross-Linking Carbon Nanotubes: a Computational Study J. Wu, A. Ayasoufi, J. Leszczynski, F.Hagelberg: J.Phys.Chem.C 117, 3646 (2013).
- (103) Density functional theory calculations of refractive indices of liquid-forming silicon oil compounds, S.Lee, S.S.Park, F.Hagelberg, Chem.Phys. 394, 40 (2012).
- (102) Do Stone-Wales Defects Alter the Magnetic and Transport Properties of Single-Walled Carbon Nanotubes? J. Wu, F. Hagelberg, T. C. Dinadayalane, D. Leszczynska, J. Leszczynski, J.Phys.Chem.C 115, 22232 (2011).
- (101) Theoretical Investigation into the Structural, Thermochemical, and Electronic Properties of the Decathio[10]circulene, B. Napolion, Frank Hagelberg, M.-J.Huang, J.D. Watts, T. M. Simeon, D. Vereen, W. L. Walters, Q. L. Williams, J.Phys.Chem A 115, 8682 (2011)
- (100) Refractive indices of liquid-forming organic compounds by density functional theory, S.S. Park, S.Lee, J. Y. Bae, Frank Hagelberg, Chem.Phys.Lett. 511, 466 (2011)
- (99) Interaction between atomic lanthanide impurities and ultra-short carbon nanotubes of the zigzag type, J.Wu, F. Hagelberg, J.Phys.Chem.C 115, 4571 (2011)
- (98) Computational approach to drying of a nanoparticle-suspended liquid droplet, H.S.Kim, S.S.Park, F.Hagelberg, J Nanopart Res. 13:59–68 (2011)
- (97) Self-assembled monolayers, F.Hagelberg, in *Handbook of Nanophysics* (volume 5: *Functional Nanomaterials*, chapter 17), ed. K.Sattler, Taylor & Francis (2010).
- (96) Structures, stabilities, and electronic properties of endo- and exohedral dodecahedral silsesquioxane (T12 – POSS) complexes with atomic and ionic species. D. Hossain, F.Hagelberg, C.Pittman, S.Saebo, Journal of Inorganic and Organometallic Polymers and Materials 20, 1574 (2010).
- (95) Adsorption of small hydrocarbon radicals on single walled carbon nanotubes of finite length. J.Wu, F. Hagelberg, Phys.Rev.B 81 155407 (2010)
- (94) Electron Transfer in Trimetal Nitride Fullerenes. F. Hagelberg, J.Wu, in: Computational Methods in Science and Engineering, AIP CP series 1148, p.702, eds.: E. Maroulis, T.E.Simos, August 2009.
- (93) Self-assembly of methanethiol on the reconstructed Au(111) surface.

G. Nenchev, B.Diaconescu, F.Hagelberg, K.Pohl, Physical Review B – Rapid Communications 80, 081401(R)(2009), ), selected for inclusion in the Virtual Journal of Nanoscale Science & Technology 20, 17 August 2009.

(92) Magnetism in finite-sized single walled carbon nanotubes of the zigzag type.  
J.Wu, F.Hagelberg, Phys. Rev. B 79, 115436 (2009)

(91) Recent Progress in the computational study of semiconductor clusters with transition metal impurities.  
J.G Han, F.Hagelberg, Journal of Computational and Theoretical Nanoscience, 6, 257 (2009).

(90) Endohedral and Exohedral Complexes of T8- Polyhedral Oligomeric Silsesquioxane (POSS) with Transition Metal Atoms and Ions.  
Delwar Hossain, Charles U. Pittman Jr., Frank Hagelberg, Svein Saebo, J.Phys.Chem.C, 112, 16070 (2008)

(89) Computational study on  $C_{80}$  enclosing mixed trimetallic nitride clusters of the form  $Gd_xM_{3-x}N$  ( $M = Sc, Sm, Lu$ ).  
J.Wu, F. Hagelberg, J.Phys.Chem.C 112, 5770 (2008).

(88)  $CH_3SH$  molecules deposited on Cu(111) and deprotonation.  
J.G.Zhou, Q.Williams, F. Hagelberg, Phys.Rev.B 77, 35402 (2008).

(87) Density Functional studies of small silicon clusters adsorbed on graphite (0001) and diamond (100), Jianhua Wu, Frank Hagelberg, Phys. Rev. B 76, 155409 (2007), selected for inclusion in the Virtual Journal of Nanoscale Science & Technology 16 October 22 2007.

(86) Headgroup dimerization in methanethiol monolayers on the Au(111) surface: A density functional theory study.  
J.G.Zhou, Q.Williams, F. Hagelberg, Phys.Rev.B 76, 75408 (2007).

(85) Structures and Stabilities of Clusters of  $Si_{12}$ ,  $Si_{18}$ , and  $Si_{20}$  Containing Endohedral Charged and Neutral Atomic Species.  
D. Hossain, F. Hagelberg, C. Pittman Jr., S. Saebo, J.Phys.Chem.C 111, 13864 (2007).

(84) Chemistry in Acetone Complexes of Metal Dications: A Remarkable Ethylene Production Pathway.  
Jianhua Wu, Dan Liu, Jian-Ge Zhou, Frank Hagelberg, Sung Soo Park, Alexandre A. Shvartsburg, J.Phys.Chem.A 111, 4748 (2007).

(83) Impact of internal electron transfer on the structure of  $C_{74}$  encapsulating Sc and La metal atom impurities.  
Dan Liu, Frank Hagelberg, Int. J. Quant. Chem. 107, 2253 (2007).

(82) Structures, stabilities, and electronic properties of exo- and endohedral complexes of T10 Polyhedral Oligomeric Silsesquioxane (POSS) cages.  
Delwar Hossain, Svein Saebo, Charles Pittman, Frank Hagelberg, J.Phys.Chem.C 111, 6199 (2007).

- (81) Electronic properties and fragmentation dynamics of organic species deposited on silicon surfaces.  
Jian-Ge Zhou, Frank Hagelberg, p.505, in: *Molecular Materials with Specific Interactions*, ed: W.A.Sokalski, Springer 2007.
- (80) Charge transfer and electron backdonation in metallofullerenes encapsulating  $\text{NSc}_3$ .  
Dan Liu, F.Hagelberg, S.S. Park, Chem. Phys. 330, 380 (2006)
- (79) Do methanethiol adsorbates on the Au(111) surface dissociate?  
Jian-Ge Zhou, Frank.Hagelberg, Phys.Rev.Lett. 97, 45505 (2006),  
selected for inclusion in the Virtual Journal of Nanoscale Science & Technology, August 7 2006.
- (78) Equilibrium geometries and associated energetic properties of mixed metal- silicon clusters from global optimization.  
J.-H. Wu , F. Hagelberg, J. Phys.Chem.A 110, 5901 (2006)
- (77) Coverage dependence of the 1-propanol adsorption on the Si(100) surface and fragmentation analysis.  
J.-G. Zhou, C.Xiao, F. Hagelberg, Phys.Rev.B 73, 155307 (2006).
- (76) Recent progress in the computational study of transition metal doped Si clusters,  
J.G. Han, F. Hagelberg, Computing Letters 1, 230 (2005).
- (75) Comparative Investigation on Non-IPR  $\text{C}_{68}$  and IPR  $\text{C}_{78}$  Fullerenes encaging  $\text{Sc}_3\text{N}$  molecules, S. S. Park, D. Liu, F. Hagelberg, J. Phys. Chem. A 109, 8865 (2005).
- (74) First principles calculations on small Silicon clusters adsorbed on a graphite surface  
J. Wu, F. Hagelberg, K. Sattler, Phys. Rev. B 72, 85441 (2005).
- (73) Free electron attachment to coronene and corannulene in the gas phase.  
S. Denifl, S.Ptasinska, B. Sonnweber, P. Scheier, D. Liu, F. Hagelberg, J. Mack, L.T. Scott, T.D. Maerk, J.Chem.Phys. 123, 104308 (2005).
- (72) Adsorption of 1-propanol on the Si(100) surface.  
J.-G. Zhou, F. Hagelberg, Int. J. Quant. Chem. 105, 3059 (2005).
- (71) Non-adiabatic Evolution of Electronic States by Electron Nuclear Dynamics Theory,  
F. Hagelberg, Int. J. Quant. Chem. 102, 869 (2005).
- (70)  $\text{Ne}_2^+[\text{II} (1/2)_u]$  : radiative decay and electronic predissociation.  
Sara Matt-Leubner, Juraj Fedor, Rajendra Parajuli, Aleksandar Stamatovic, Olof Echt, Frank Hagelberg, Krzysztof Gluch, Michael Probst, Paul Scheier, Tilmann D. Märk, Phys.Chem.Chem.Phys. 7, 1043 (2005).
- (69) Endohedral and Exohedral Complexes of Polyhedral Double Four-Membered Ring (D4R) Units with Atomic and Ionic Impurities.

Sung Soo Park, Chuanyun Xiao, and Frank Hagelberg, Delwar Hossain, Charles U. Pittman, Jr., Svein Saebo, *J. Phys. Chem. A* 108, 11260 (2004).

(68) Formation and Unimolecular Dissociation of  $\text{Al}^{3+}(\text{DMSO})_n$  Complexes.  
Ahmed M. El-Nahas, Chuanyun Xiao, Frank Hagelberg, *Int. J. Mass Spec.* 237, 47 (2004).

(67) A Density-functional study on the structures, stabilities and dissociation pathways of  $\text{Sc}^{3+}(\text{DMSO})_n$  complexes ( $n=1-6$ ).  
C. Xiao, F. Hagelberg, A. M. El-Nahas, *J. Phys. Chem. A* 108, 5322 (2004).

(66) Theoretical study on the structures and dissociation channels of metal dications solvated by acetonitrile ligands.  
C. Xiao, K. Walker, F. Hagelberg, A. M. El-Nahas, *Int. J. Mass Spec.* 233, 87 (2004).

(65) Silicon clusters doped with an Yttrium metal atom.  
C. Xiao, J. Blundell, F. Hagelberg, W. A. Lester, Jr., *Int. J. Quant. Chem.* 96, 461 (2004).

(64) Probing electronic states of  $\text{Ne}_2^+$  and  $\text{Ar}_2^+$  by measuring kinetic-energy-release distributions.  
J. Fedor, R. Parajuli, S. Matt-Leubner, O. Echt, F. Hagelberg, K. Gluch, M. Probst, P. Scheier, T. D. Maerk., *Phys. Rev. Lett.* 91, 133401 (2003).

(63) The Formation of New Silicon Cages: A Semiempirical Theoretical Investigation.  
J. G. Han, Z. Y. Ren, Z. F. Chen, L. S. Sheng, Y. W. Zhang, J. A. Morales and F. Hagelberg, *J. Mol. Struct. (Theochem)* 625, 47 (2003)

(62) Energetics and dynamics of decaying cluster ions.  
K. Gluch, J. Fedor, S. Matt-Leubner, R. Parajuli, C. Mair, A. Stamatovic, O. Echt, C. Lifshitz, J. Harvey, F. Hagelberg, Z. Herman, M. Probst, P. Scheier, T. D. Maerk, *Eur. Phys. J. D* 24, 131 (2003).

(61) Cage-like  $\text{Si}_{12}$  Clusters with Endohedral Cu, Mo and W Metal Atom Impurities.  
F. Hagelberg, C. Xiao, W. A. Lester, Jr., *Phys. Rev. B* 67, 035426 (2003).

(60) Computational Study of  $\text{IrSi}_9^+$  Isomers.  
F. Hagelberg, C. Xiao, *Struct. Chem.* 14, 487 (2003).

(59) Comparative study on the interaction of Sc and Cu atoms with small silicon clusters.  
C. Xiao, A. Abraham, R. Quinn, F. Hagelberg, W. A. Lester, Jr., *J. Phys. Chem.* 106, 11380 (2002)

(58) Geometric, Energetic and Bonding Properties of Neutral and Charged Copper-Doped Silicon Clusters.  
C. Xiao, F. Hagelberg, W. A. Lester, Jr., *Phys. Rev. B* 66, 75425 (2002).

(57) Isotope Effects in the Electron Impact Ionization of  $\text{H}_2/\text{D}_2$ ,  $\text{H}_2\text{O}/\text{D}_2\text{O}$  and  $\text{C}_6\text{H}_6/\text{C}_6\text{D}_6$  near Threshold.  
G. Hanel, B. Gstir, T. Fiegele, F. Hagelberg, K. Becker, P. Scheier, A. Snegursky, T. D. Maerk, *J. Chem. Phys.* 116, 2456 (2002).



- (56) Non-adiabatic Effects in the Pseudorotational Motion of Triatomic Molecules.  
F.Hagelberg, E.Deumens, Phys.Rev.A. 65, 52505 (2002).
- (55) Hartree-Fock calculations for FeCl<sub>2</sub> and FeBr<sub>2</sub> – the question of the <sup>57m</sup>Fe quadrupole moment.  
F.Hagelberg, T.P.Das, K.C.Mishra, Phys.Rev.B 65 14425 (2002).
- (54) Geometric and electronic structure of WSi<sub>n</sub> (n=1-6,12) clusters.  
J.-G. Han, C.Xiao, F.Hagelberg, Struct. Chem. 13(2) 173 (2002)
- (53) Pseudorotational Dynamics of H<sub>3</sub><sup>+</sup> and Li<sub>3</sub><sup>+</sup>.  
F. Hagelberg, Int.J. Quant.Chem. 85, 72 (2001)
- (52) Theoretical study of small silicon clusters on a graphite layer.  
F.Hagelberg, C.Xiao, B.Marsen, M.Lonfat, P.Scheier, K.Sattler, Eur.Phys.J.D 16, 37 (2001)
- (51) A density functional investigations of MoSi<sub>n</sub> (n = 1-6) clusters.  
Ju-Guang Han, Frank Hagelberg, J.Molec.Struct. (Theochem) 549, 165 (2001)
- (50) Quantum Monte Carlo characterization of small Cu-doped silicon clusters: CuSi<sub>4</sub> and CuSi<sub>6</sub>.  
I.V.Ovcharenko, W.A.Lester,Jr., C.Xiao, F.Hagelberg, J.Chem.Phys. 114, 9028 (2001).
- (49) Geometric structures and stabilities of CuSi<sub>n</sub> clusters (n = 8, 10, 12).  
C.Xiao, F.Hagelberg, I.Ovcharenko, W.A.Lester,Jr., J.Molec.Struct. (Theochem) 549,181 (2001).
- (48) Formation and dissociation of triply charged fragment ions of benzene.  
F.Scheuermann, E.Salzborn, F.Hagelberg, P.Scheier, J.Chem.Phys. 114, 9875 (2001).
- (47) A density functional theory investigation on CrSi<sub>n</sub> (n=1-6) Clusters.  
J.G.Han, F. Hagelberg, Chem.Phys. 263, 255 (2001)
- (46) Coulomb blockade effects in charged Si<sub>7</sub> clusters on a graphite substrate.  
F.Hagelberg, P.Scheier, B.Marsen, M.Lonfat, K.Sattler, J.Molec.Struct.(Theochem) 529, 149 (2000).
- (45) Pseudoprecession of Triatomic Systems by Electron Nuclear Dynamics Theory.  
F. Hagelberg, Int.J.Quant.Chem. 80, 966 (2000)
- (44) Spin Transfer as Stabilization Mechanism in Arsenic Based Zintl Clusters.  
D.Spencer, F. Hagelberg, J.Molec. Struct., J.Molec.Struct.(Theochem) 529, 259 (2000).
- (43) Computational Studies on Si<sub>7</sub> Clusters Deposited on a Graphite Substrate.  
F.Hagelberg, P.Scheier, B.Marsen, M.Lonfat, K.Sattler, in: "Cluster and Nanostructure Interfaces". Eds.: P.Jena, S.N.Khanna, B.K.Rao, eds., World Scientific, Singapore 2000, 619.

- (42) Charge Transfer Mechanism in Cu-doped Silicon Clusters: A Density Functional Study.  
C. Xiao, F.Hagelberg, J.Molec.Struct. (Theochem) 529, 241 (2000).
- (41) Electron Nuclear Dynamics Studies of H<sub>3</sub> and H<sub>3</sub><sup>+</sup>.  
F. Hagelberg, Int.J.Quant.Chem. 75, 367 (1999).
- (40) Quantum dynamical studies of H<sub>3</sub>.  
F.Hagelberg, J.Molec.Struc. (Theochem) 487, 151 (1999).
- (39) Theoretical Investigations on closed-shell silicon clusters doped with Cu atoms.  
F.Hagelberg, I.Yanov, J.Leszczynski, J.Molec.Struc.(Theochem) 487, 183 (1999).
- (38) Transient Field Measurement in the giant moment PdFe alloy  
B.Heller, K.-H.Speidel, R.Ernst,A.Gohla, U.Grabowy, U.Roth, G.Jakob,  
F.Hagelberg, J.Gerber, S.N.Mishra, P.N.Tandon, Nuc.Inst.Meth. B 142 133 (1998).
- (37) Evaluation of the <sup>57</sup>Fe Quadrupole Moment from Hartree – Fock Calculations.  
F.Hagelberg, T.P.Das, Z.Naturforsch.53a, 358 (1998).
- (36) Theoretical Investigations on Small Closed – Shell Silicon<sub>N</sub> Clusters.  
F.Hagelberg, J.Leszczynski, V.Murashov, A.Korkin, J.Molec.Struc.(Theochem) 454, 209 (1998).
- (35) Zintl Clusters analogous to Ozone.  
F.Hagelberg, T.P.Das, K.G.Weil, J.Phys.Chem.102, 4630 (1998).
- (34) Synchrotron White Beam Thermal Loading of Polycapillary X-Ray Optic.  
B.K.Rath, F.Hagelberg, B.E.Honan, C.A.MacDonald, Nucl.Instr.Meth.A, 401, 421 (1997)
- (33) Electric Field Gradients for Small Antimony based Zintl Clusters from Hartree-Fock Investigations.  
F.Hagelberg, T.P.Das, K.G.Weil, Z. Naturforsch.51a, 557 (1996).
- (32) Spin Exchange between Fast Ions and Majority Electrons in Ferromagnets as the Origin of Transient Fields.  
F. Hagelberg, T.P.Das, K.-H.Speidel, Hyperfine Interactions C 1, 151 (1996).
- (31) Theory of Electric Field Gradients for Sb<sub>4</sub> - and Sb<sub>4</sub><sup>2-</sup> analogous Zintl Clusters.  
F.Hagelberg, T.P.Das, K.G.Weil, Hyperfine Interactions C 1, 13 (1996).
- (30) Ab Initio Investigations on Sb<sub>4</sub> analogous Zintl Clusters.  
F.Hagelberg, Sudha Srinivas, N.Sahoo, T.P.Das, K.G.Weil , Phys.Rev.A 53, 353 (1996).
- (29) On the Origin of Transient Magnetic Fields.  
F.Hagelberg, in: Proceedings of the Symposium on Local Order in Condensed Matter Physics, eds. P.Jena, S.Mahanti and B.K.Rao, Nova Science Publishers, New York (1995).

- (28) Hyperfine Interaction Studies on swift O-ions emerging emerging with Polarized Electrons from Ferromagnetic Layers into Vacuum.  
S.Kremeyer, K.-H.Speidel, O.Jessensky, H.Busch, U.Grabowy, A.Gohla, J.Cub, G.Jakob, P.Maier-Komor, J.Gerber, A.Meens, F.Hagelberg, T.P.Das,Z.Phys.A 348, 49 (1994).
- (27) Structure and Bonding in Alkali-Antimony ( $A_nSb_4$ ) Clusters .  
F.Hagelberg, S.Neeser, N.Sahoo, T.P.Das, K.G.Weil, Phys. Rev.A 50, 557 (1994).
- (26) Theory of Location and Associated Hyperfine Properties of Positive Muon in  $La_2CuO_4$ .  
S.B.Sulaiman, Sudha Srinivas, N.Sahoo, F.Hagelberg, T.P.Das, E.Torikai, K.Nagamine, Phys.Rev.B 49, 9879 (1994).
- (25) Spin Exchange Scattering between Fast Ions and Localized Moments in Ferromagnets as the Origin of Transient Fields.  
F.Hagelberg, T.P.Das and K.-H.Speidel, Phys.Rev.C 48, 2230 (1993).
- (24) Theory of Location and Associated Hyperfine Properties of Positive Muon in High- $T_c$  Systems.  
S.B.Sulaiman, N.Sahoo, Sudha Srinivas, F.Hagelberg, E.Torikai and K.Nagamine, Hyperfine Interactions 79, 901 (1993).
- (23) First Principles Theory for Location of Positive Muon in  $La_2CuO_4$  and Associated Hyperfine Interactions.  
S.B.Sulaiman, N.Sahoo, F.Hagelberg, Sudha Srinivas, E.Torikai, K.Nagamine, Hyperfine Interactions 79, 739 (1993).
- (22) Theory for Position of Muon in  $\alpha$ -Quartz and Associated Hyperfine Interaction.  
S.M.Mohapatra, N.Sahoo, K.C.Mishra, Tina Briere, Sudha Srinivas, F.Hagelberg, Hyperfine Interactions 79, 659 (1993).
- (21) Transient Field Measurements on  $^{32}S(2+)$  Ions in Gd at the 1s Electron Bohr Velocity.  
J.Cub, M.Bussas, K.-H.Speidel, W.Karle, U.Knopp, H.Busch, H.-J.Wollersheim, J.Gerl, K.Vetter, C.Ender, F.Koeck, J.Gerber, F.Hagelberg, Z.Phys.A 345, 1 (1993).
- (20) Hartree-Fock Investigations of Electronic Structure and  $^{19}F^*$  Quadrupole Interactions in Fluorobenzenes.  
S.Swingle-Nunes, N.Sahoo, F.Hagelberg, T.P.Das, K.Bonde Nielsen, J. Am. Chem. Soc. 115, 5145 (1993).
- (19) Hartree-Fock Investigation of the Structure of  $Sb_4$  Clusters.  
F.Hagelberg, N.Sahoo, T.P.Das, K.-G.Weil, K.-H.Speidel, Phys.Rev.A46, 6087 (1992).
- (18) New Determination of the Magnetic Moment of the  $^{54}Fe(2+)$  State at 1.408 MeV. K.-H.Speidel, J.Cub, U.Reuter-Knopp, W.Karle, H.Busch, S.Kremeyer, J.Gerber, F.Hagelberg, Z.Phys.A 342, 17 (1992).

- (17) Hartree-Fock Investigation of Pure Antimony and Alkali-Antimony Clusters. F.Hagelberg, S.Neeser, N.Sahoo, T.P.Das, K.G.Weil, K.-H.Speidel, in: Physics and Chemistry of Finite Systems: From Clusters to Crystals, Editors: P.Jena, S.N. Khanna, B.K.Rao, Kluwer Academic Publishers, Dordrecht (1992).
- (16) Electron Polarization of Highly Stripped Oxygen Ions Emerging from Magnetized Iron Layers. H.-J.Simonis, S.Kremeyer, U.Reuter, F.Hagelberg, G.-M.Kim, K.-H. Speidel, M.Knopp, J.Cub, W.Karle, M.Weidinger, J.Gerber, A.Meens, P.N.Tandon, Phys.Lett.B 254 No.1,2 35 (1991).
- (15) Plunger Measurements on Highly Stripped O-Ions as Tool for Detecting Electron Polarization on Emergence from Thin Ferromagnetic Layers. H.-J.Simonis, S.Kremeyer, F.Hagelberg, U.Reuter, M.Knopp, K.-H.Speidel, J.Cub, W.Karle, P.N.Tandon, J.Gerber, Hyperfine Interactions 61, 1347 (1990).
- (14) Spin Exchange Scattering as the Most Likely Polarization Mechanism in Transient Magnetic Fields. F.Hagelberg, K.-H.Speidel, P.N.Tandon, Z.Phys.D17, 17 (1990).
- (13) Transient Magnetic Fields for Highly Stripped Ions Traversing Ferromagnetic Solids. K.-H.Speidel, M.Knopp, W.Karle, J.Cub, M.-L.Dong, H.-J.Simonis, F.Hagelberg, U.Reuter, S.Kremeyer, J.Gerber, Hyperfine Interactions 51, 817 (1989).
- (12) Large Transient Magnetic Fields for Single-Electron O-Ions on a 10fs Time Scale. U.Reuter, F.Hagelberg, S.Kremeyer, H.-J.Simonis, K.-H.Speidel, M.Knopp, W.Karle, J.Cub, J.Gerber, Phys.Lett. B230 No.1,2 16 (1989).
- (11) Measurement of Lifetime and g-Factor of the  $^{32}\text{S}(4+)$  State at 4.459 MeV. H.-J.Simonis, F.Hagelberg, K.-H.Speidel, M.Knopp, W.Karle, U.Kilgus, J.Gerber, Z.Phys.A330, 361 (1988).
- (10) Evidence for Spin Polarized Electrons of Highly Stripped Fluorine Ions Emerging from Thin Ferromagnetic Layers. K.-H.Speidel, M.Knopp, W.Karle, P.Maier-Komor, H.-J.Simonis, F.Hagelberg, J.Gerber, P.N.Tandon, Phys. Rev. Lett. 61,22, 2616 (1988).
- (9) New Aspects in Transient Magnetic Fields Using Heavy Ion Beams. K.-H.Speidel, M.Knopp, W.Karle, U.Kilgus, M.-L.Dong, H.-J.Simonis, F.Hagelberg, J.Gerber, Z.Phys.A331, 29 (1988).
- (8) Attenuations and Atomic Spin Precessions of  $\gamma$ -Angular Correlations for Coulomb Excited  $^{19}\text{F}$  Nuclei in Single Electron Ions. M.Knopp, K.-H.Speidel, F.Hagelberg, H.-J.Simonis, P.N.Tandon, J.Gerber, Z.Phys.D4, 329 (1987).
- (7) Transient Field Precessions and Electron Polarizations for Sulphur Ions at High Velocity.

H.-J.Simonis, F.Hagelberg, M.Knopp, K.-H.Speidel, W.Karle, J.Gerber, Z.Phys.D7, 233 (1987).

(6) Measurements of the g-Factor Ratio of the first 3- and 5- states in  $^{40}\text{Ca}$  and the lifetime of the 5- state.

M.Mayr, K.-H.Speidel, M.Knopp, W.Karle, T.Faestermann, F.Hagelberg, H.-J.Simonis, P.N.Tandon, J.Gerber, Z.Phys.A327, 157 (1987).

(5) The Effect of Helium Layers Implanted into Thin Iron Foils on Transient Magnetic Fields.

H.-J.Simonis, F.Hagelberg, W.Troelenberg, K.-H.Speidel, M.Knopp, J.Gerber, Nucl. Instr. Meth. B21, 56 (1987).

(4) Transient K-shell Hyperfine Fields and Deduced Polarizations for Single Electron C and O Ions in Different Ferromagnets.

K.-H.Speidel, M.Knopp, W.Karle, M.Mayr, F.Hagelberg, H.-J.Simonis, J.Gerber, P.N.Tandon, Z.Phys.D6, 43 (1987).

(3) Transient Magnetic Fields at Ne Ions in Fe and Gd Hosts and a Critical Assessment of  $^{20}\text{Ne}(4+)$  g-Factor Measurements.

W.Troelenberg, F.Hagelberg, H.-J.Simonis, P.N.Tandon, K.-H.Speidel, M.Knopp, J.Gerber, Nucl.Phys.A458, 95 (1986).

(2) Strong Enhancement of Transient Magnetic Fields in Gd over Fe for Oxygen Ions at High Velocities.

K.-H.Speidel, F.Hagelberg, M.Knopp, W.Troelenberg, H.Neuburger, J.Gerber, S.S. Hanna, H.Dekhissi, P.N.Tandon, Z.Phys.D1, 363 (1986).

(1) Atomic Spin Precessions of Fluorine Ions Recoiling Through Vacuum in Weak Transverse Magnetic Fields.

M.Knopp, V.Mertens, F.Hagelberg, K.-H.Speidel, J.Gerber, H.Dekhissi, P.N.Tandon, Z.Phys. A320, 635 (1985).