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Education

1985 B.Sc. (Physics) University of Toronto, Canada
1988 M.Sc. (Physics) Queen's University at Kingston, Canada
1992 Ph.D. (Physics) Queen's University at Kingston, Canada

Professional Career (Arizona State University)

2007–present Associate Professor, Department of Chemistry and Biochemistry,
2006–present Affiliated Professor, Department of Physics and Astronomy,
2001–2006 Associate Research Scientist, Center for Solid State Science,
Affiliated Faculty, Science and Engineering of Materials Graduate Program,
1998–2006 Manager, Goldwater Materials Visualization Facility,
Center for Solid State Science
1998-2001 Academic Associate, Center for Solid State Science,
1996–1998 Education Coordinator, Materials Research Science & Engineering Center,
1994–1996 Faculty Research Associate, Department of Chemistry and Biochemistry,
1992–1996 Visiting Scientist, Department of Chemistry and Biochemistry,

Professional Memberships

Materials Research Society
American Physical Society
American Geophysical Union
Canadian Association of Physicists

Research Specialization

Theory: Density functional theory and *ab initio* quantum chemistry simulation of optical, vibrational, electronic and thermoelastic properties solids, gases and liquids. Current research interests include prediction of water-silica exoplanetary geochemistry, water and nitrogen in earth's mantle, new superhard nitrogen-based materials, novel non-linear optical materials.

Experiment: Expertise in spectroscopic in situ characterization of high-pressure supercritical behavior of water, CO₂, their mixtures, and their fundamental interactions with mineral systems. Innovator in the application of in situ techniques in CO₂ sequestration via direct mineralization, and in the context of geological storage.

Professional activities and Services

SMS Committees and Services (**2016**): Committee on Undergraduate Programs
Search Committee (SMS/CAMD)
Search Committee (SMS Molecular Design Biomimetics)

ASU Committees and Services (**2016**): Member, ASU Working Group for Research Computing
University Senator (SMS)
CLAS Senator (SMS)
Associate Director, PSM in Nanoscience Program

2008-present Undergraduate Programs Committee: (Dept of Chemistry/Biochemistry – ASU)

1999–present *Proposal Reviewer/Panelist:* Department of Energy (SciDAC, University Coal Research, Fossil Energy, BES), Petroleum Research Fund, National Science Foundation (DMR, Geochemistry, CTS, CBET), Alberta Ingenuity Fund, Oak Ridge Inst. Sci. Ed. (ORISE), Austrian Science Fund

1994–present *Publication Referee:* Physical Review Letters, Physical Review B, Journal of Chemical Physics, Chemistry of Materials, Environmental Science and Technology, Acta Materialia, Applied Physics Letters, Environmental Science and Technology, Microscopy and Microanalysis, Journal of the Electrochemical Society, Energy and others.

2009-2015 Chair, Computing Committee, (Dept. of Chemistry and Biochemistry – ASU)

1998–2014 Registered Synchrotron, Argonne National Laboratory & Core Radiological certification (USDOE)

- 2006-2013 Conference committee member, International Technical Conference on Coal Utilization and Fuel Systems
- 1998–2013 A founding member of the National Mineral Sequestration Working Group (managed by the U.S. Department of Energy)
- 2006-2011 Fulton High Performance Computing Initiative Advisory Committee (ASU)
- 2006-2007 Computing Resources Committee, (Dept of Chemistry/Biochemistry – ASU)
Awards Committee, (Dept of Chemistry/Biochemistry – ASU)
- 2007-2008 Strategic Planning: Chemistry of Global Sustainability Committee, (Dept of Chemistry/Biochemistry – ASU)

Teaching experience

- Undergraduate: CHM 346 Physical Chemistry II (Thermodynamics)
CHM 341 Elementary Physical Chemistry (Thermo, Stat Mech, Quantum)
CHM 240 Introduction to Physical Chemistry (Mathematical Methods)
CHM 501 Current Topics in Chemistry (Student and Guest Presentations)
- Graduate: CHM 543 Computational Chemistry (External speakers, Lectures and Lab)
NAN 591 Nanotechnology (Student Seminars, Lectures by Instr. & Speakers)

Graduate Committee Service (2016):

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| Ph.D. Comprehensive Exam Committee Chair:
Parker Castleberry, SMS (04/01/16) | Ph.D. Technical Review Committee Member:
Lasitha Senaratne, SMS (02/15/16)
Andrew Copple, Physics (02/05/16) |
| Ph.D. Comprehensive Exam Committee Member:
Morteza M. Waskasi, SMS (01/15/16)
Trunk Nguyen, SMS (03/16/16)
Ehsan Gharib Nezhad, SMS (03/18/16) | Ph.D. Examination Committee Member:
Lasitha Senaratne, SMS (06/15/16)
Andrew Copple, Physics (06/19/16) |

Mentoring Activities (2001-present):

Post-doctoral Advisor:

Jason Diefenbacher (2010-2013)
Hamdallah Bearat (2006-2010)
Naoki Ito (2006-2010)
Po-Liang Liu (2004-2005)
Jason Diefenbacher (2001-2005)

Graduate Advisor:

Robert Allan (Ph.D. 2016-present)
Cliff Ghiglieri (M.Sc. PSM Nanoscience, 2015-2016)
Deirdre Gormley (Ph.D., 2001-2005)(now at Johnson&Johnson)
Michael Kocher (M.Sc., 2002-2004)(ASU SEM program)
Renee Olsen (M.Sc., 1999-2002)(now at Lockheed- Martin)

Graduate co-Advisor:

Narges Masoumi (Ph.D. 2015-present)
Ganesh Subramanian (Ph.D. 2016)
Patrick Sims (Ph.D. 2012)
Tylan Watkins (Ph.D., 2010-2012)
Justin Spiriti (Ph.D., 2009-2011)
Change Weng (Ph.D., 2008-2010)
Ravi Shivaraman (M.Sc. 2006-2008)

Undergraduate Advisor:

Spencer Hall (SMS Spring 2016)
Michael Rozowski (Chemistry summer 2015)
James Gallagher (Physics spring 2013)
Beth Denton (ORICA Research Assistant, 2009-2011)
Monika Ciuba (ASU Undergraduate Scholar, 2007-2008)
Meredith Reitz (Honors Thesis, 2007)
Katrin Passlack (Honors Thesis, 2006)
Kris Rademacher, Brian Pang, Reddy Takulapalli, Asif Kahn

Recent Invited/Contributed Talks and Presentations

"*First Principles Design of Silicon-compatible Si₂AlP alloy Absorber Materials: Optical Tuning via Nanostructure*" A.V.G. Chizmeshya, Materials Research Society Fall Meeting, Boston MA, November 29 (2016).

"*Comparative Study of the Structural, Electronic and Thermoelastic Properties SiO₂ and Si(NH)₂ from First Principles*" N. Masoumi, G.H. Wolf and A.V.G. Chizmeshya, Materials Research Society Fall Meeting, Boston MA, November 29 (2016).

"*Fundamental Studies of Clay and Clay-rich Mineral Reactions with H₂O-CO₂ Fluids: Application to Geological Carbon Dioxide Sequestration*", Andrew V.G. Chizmeshya, Fall Meeting of the American Geophysical Union, San Francisco CA, December 15 (2016).

"Characterizing the Intermediate State Electronic and Molecular Structure during the Photolysis of Methylcobalamin, using Ultrafast Pump-probe X-ray Absorption Spectroscopy", G. Subramanian, G. Kodis, G. Zhang, Q. Kong, A.V.G. Chizmeshya and J.C.H. Spence, 3rd International BioXFEL Conference, San Juan, Puerto Rico, January 12 (2016).

"Perspective on Engineering the Fate of Fossil-based CO₂: Conversion to Mineral Carbonate vs Below-ground Injection", (Invited) Andrew V.G. Chizmeshya, ASU Center for Negative Carbon Emissions, Host: Klaus Lackner, April 1 (2016).

"In Situ Studies of 'Mineral-CO₂' Interactions relevant to Carbon Sequestration", (Invited) Andrew V.G. Chizmeshya, 5th International Conference on Accelerated Carbonation for Environmental and Material Engineering, Host: Prof. Alissa Park, New York NY, June 23 (2015).

"Physics and Chemistry Simulations from First Principles: Methodologies, capabilities and applications to new materials systems", (Invited) Andrew V.G. Chizmeshya, Northrop Grumman Nanotechnology Workshop, Host: Dr. J. Tice, Redondo Beach CA, July 7 (2015).

"New GeSi doping strategies based on P(SiH₃)₃ for next-generation CMOS technologies" Annual March APS Meeting (International), San Antonio TX, March 4 (2015).

"Structural and Thermochemical Aspects of (III-V)IV₃ Material Assembly from First Principles" Andrew V.G. Chizmeshya and John Kouvetakis, American Physical Society March Meeting, Denver, Colorado, March 6 (2014).

"In Situ Studies of Mineral-CO₂ Interactions relevant to Carbon Sequestration" Andrew V.G. Chizmeshya, (Invited), Lenfest Center for Sustainable Energy, Earth Institute at Columbia University, New York NY, Host: Prof. Klaus Lackner, March 25 (2013).

"Fundamental Studies of Clay and Clay-rich Mineral Reactions with H₂O-CO₂ Fluids: Applications to Geological Sequestration" (Invited), Andrew V.G. Chizmeshya, National Energy Technology Laboratory, Pittsburgh PA, Host: Dr. Andrea Dunn, October 30 (2012).

"Nano-synthesis Approach to the Fabrication of Monocrystalline Silicon-like (III-V)_yIV_{5-2y} Semiconductors" A.V.G. Chizmeshya, ECS-PRIME – Pacific Rim Meeting on Electrochemical and Solid-state Science, Honolulu, Hawaii, October 12 (2012).

"Chemistry of Sustainable Fossil Fuel Utilization" Andrew V.G. Chizmeshya, Department of Chemistry and Biochemistry, Arizona State University, Tempe AZ. Graduate Seminar Host: Prof. A. Angell, January 26 (2012).

"CO₂ Sequestration in a Carbon Constrained Future" Andrew V.G. Chizmeshya, *Invited Colloquium* School of Earth Science and Exploration (SESE), Arizona State University, Tempe, AZ. Host: Prof. P. Buseck, April 13 (2011).

"Chemistry of Sustainable Fossil Fuel Utilization" Andrew V.G. Chizmeshya, Department of Chemistry and Biochemistry, Arizona State University, Tempe AZ. Host: Prof. A. Angell, February 26 (2011).

"Theory of SiSn Alloys", A.V.G. Chizmeshya, Air Force Office of Scientific Research Nanophotonics Program Review Meeting, Cambridge MA. Host: Dr. Gernot Pomrenke December 1, (2010).

"Optical Properties and Theoretical Simulations of Si-N-P Alloys", A.V.G. Chizmeshya, Air Force Office of Scientific Research Nanophotonics Program Review Meeting, Cambridge MA. Host: Dr. Gernot Pomrenke, December 1, (2010).

"In Situ CO₂ Sequestration Reaction Studies in above Ground and Geological settings", Invited talk, National Energy Technology Laboratory, Pittsburgh, PA. Host: Dr. George Guthrie, April 29, (2010)

"Practical Strategies for Tuning Optical, Structural and Thermal Properties of Group IV Ternary Semiconductors" J. Kouvetakis and A.V.G. Chizmeshya, Fourth International SiGe, Ge, & Related Compounds Symposium (ECS Conference), Las Vegas NV, October 14, (2010).

"CO₂ Sequestration via Mineralization: In Situ Reaction Studies in Above Ground and Geological setting" Andrew V.G. Chizmeshya, *Shell Global Solutions International BV*, 1030 BN Amsterdam, The Netherlands. Host: Dr. Marcel Verduyn, January 21 (2009).

"Chemistry of Sustainable Fossil Fuel Utilization" Andrew V.G. Chizmeshya, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ. Host: Prof. A. Angell, March 12 (2009).

"*In Situ* Mineral Sequestration Reaction Studies in 'Above Ground' and Geological setting" A.V.G. Chizmeshya, 2nd U.S.-China Symposium on CO₂ Emissions Control Science & Technology, Hangzhou, China. Host: Dr. Zhongyang Luo, Zhejiang University May 29 (2008).

"CO₂ Sequestration via Mineralization: Recent advances in the *in situ* investigation of geological reactions" Andrew V.G. Chizmeshya, Hamdallah Béarat, George H. Wolf, Robert Marzke, Naoki Ito, and Brandon Doss. 33rd International Technical Conference on Coal Utilization & Fuel Systems, Clearwater, Florida. Host: Barbara Sakestaad, June 5, (2008).

"CO₂ Sequestration via Mineralization: *In Situ* Reaction Studies in 'Above Ground' and Geological setting" A.V.G. Chizmeshya, Lawrence Livermore National Laboratory, Livermore, California (2008). Host: Dr. Julio Friedman, Director Carbon Management, July 22, (2008).

"First principles Simulations of Optical, Electronic and Structural Properties of Si-Ge-Sn alloys" A.V.G. Chizmeshya, Nano-structure and Nano-photonics MURI Meeting, Boston, MA: Host: Dr. G. Pomrenke, 30 November (2007).

"Energy Strategies in a Carbon Constrained World: Carbon Sequestration and New Alternative Energy Strategies" A.V.G. Chizmeshya, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ. Host: Prof. A. Angell, September 12 (2007).

"Nanomaterials Simulation using High Performance Computing: From Greenhouse Gases to High-Tech Materials" A.V.G. Chizmeshya (presenter) and D. Stanzione, 2nd IEEE/ACM International Workshop on High Performance Computing for Nano-science and Technology, 19th International Conference for High Performance Computing, Tampa, FL. Host: Dr. Jun Ni (Iowa State U.), November 13 (2006).

"Adventures in Computational Materials Chemistry" A.V.G. Chizmeshya, Departmental Colloquium, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ. Host: Prof. W.T. Petuskey, April 17 (2006).

"CLEAN CONSUMPTION OF FOSSIL FUELS in the 21st CENTURY: CARBON SEQUESTRATION", A.V.G. Chizmeshya, Arizona State University, Tempe, AZ. Host: F. DiSalvo (Visiting Prof), February 14 (2006).

"Simulation, Visualization and Predictive Modeling in Materials Science and Engineering", A.V.G. Chizmeshya ASM Arizona "Materials Advantage" Chapter, Arizona State University, Tempe, AZ. Host: E. Engstrom, October 4 (2005).

"Simulation, Visualization and Predictive Modeling at the Atomic and Molecular Scale", A.V.G. Chizmeshya Invited Lecture (History and Philosophy of Science), Arizona State University, Tempe, AZ. Host: Prof. T. Martin, April 5 (2005).

"Quantitative Prediction of Interaction Potentials for Weak Binding Systems: Inert gases on cold surfaces", A.V.G. Chizmeshya, Departmental Colloquium (Physics), University of Arizona, Tucson, AZ. Host: Prof. A. Cronin, January 23 (2005).

"Furthering the Mechanistic Understanding of Above-Ground CO₂ Mineral Sequestration Reaction Processes" McKelvy, M.J., Chizmeshya, A.V.G., Diefenbacher, J., Bearat, H., Carpenter, R.W., and Wolf G.H., 30th International Technical Conference on Coal Utilization & Fuel Systems (04/2005).

"Developing an atomic-level understanding of the mechanisms that govern CO₂ sequestration mineral carbonation reaction processes", McKelvy, M.J.; Chizmeshya, A.V.G.; Diefenbacher, J.R.; Bearat, H.; Carpenter, R.W.; Wolf, G.H.; Gormley, D., TMS Annual Meeting: EPD Congress (Invited Presentation) (02/2005).

"Structure of Low-Loss EELS in Rhenium", Carpenter R.W. and Chizmeshya A.V.G., 2005 Microscopy Society of America Meeting: Microscopy and Microanalysis, (07/2005).

"The Nanoscale Mechanism for San Carlos Olivine Carbonation", Kim, Y.-C.; Nunez, R.; Carpenter, R.W.; Chizmeshya, A.V.G.; McKelvy, M.J. 2005 Microscopy Society of America Meeting: Microscopy and Microanalysis (07/2005).

"Lamellar Reaction Phenomena: from Intercalation to Nanomaterials Formation", M.J. McKelvy, A.V.G. Chizmeshya and R. Sharma, 13th International Symposium on Intercalation Compounds (06/2005).

"Enhancing the Atomic-Level Understanding of CO₂ Mineral Sequestration Mechanisms via Advanced Computational Modeling", A.V.G. Chizmeshya, University Coal Research/Historically Black Colleges and Universities Meeting, Pittsburgh, PA. Host: Dr. John Litinsky, July 17 (2004).

"Recent Advances in CO₂ Sequestration by Mineral Carbonation: Experiments and Theory" A.V.G. Chizmeshya, Departmental Colloquium (Chemistry), Lehigh University, Bethlehem, PA. Host: Prof. K. Klier, November 10 (2004).

"Quantitative Prediction of Interaction Potentials for Weak-Binding Systems Departmental Seminar", A.V.G. Chizmeshya, Departmental Seminar (Physics), Pennsylvania State University, College Park, PA. Host: Prof. M.W. Cole, November 9 (2004).

"CO₂ mineral carbonation processes in olivine feedstock: insights from the atomic scale simulation" Chizmeshya, Andrew V. G.; McKelvy, Michael J.; Gormley, Deirdre; Nunez, Ryan; Kim, Youngchul; Carpenter, Ray. 29th Coal Utilization and Fuel Systems Conference, Host: B. Sakkestad, Clearwater Florida, April 22 (2004).

"IR Semiconductors in the Si-Ge-Sn System" J. Kouvetakis, J. Menendez, J. Tolle, A.V.G. Chizmeshya and C. Ritter, First International Silicon Photonics Conference, Hong Kong (2004).

"Synthesis of IR and UV optical materials using molecular chemistry", J. Kouvetakis, J. Tolle, A. Chizmeshya, M. Bauer, and J. Menendez, Institute of Physics, Academia Sinica, Prague, Czech Republic (2004).

"Mechanistic and Computational Study of Cinnabar Phase Transformation : Applications and Implications to The Preservation of This Pigment in Historical Paintings", H. Bearat, A. Chizmeshya, R. Sharma, A. Barbet, and M. Fuchs, The Third International Conference on Science and Technology in Archaeology and Conservation, Israel (2004).

"Exploration of the role of heat activation in enhancing serpentine carbon sequestration reactions", McKelvy, Michael J.; Chizmeshya, Andrew V. G.; Diefenbacher, Jason; Bearat, Hamdallah; Wolf, George 29th Coal Utilization and Fuel Systems Conference, Clearwater Florida Contributed Colloquia International 04/2004 Y co-author

"Quantum Simulation Studies of Olivine Mineral Carbonation" Andrew V.G. Chizmeshya, Michael J. McKelvy, George H. Wolf, Renu Sharma, Otto F. Sankey, Hamdallah Bearat, Jason Diefenbacher, and R.W. Carpenter, 27th International Technical Conference on Coal Utilization & Fuel Systems, Host: B. Sakkestad, Clearwater, Florida, March 1 (2003).

"CO₂ Mineral Sequestration: An Opportunity for Materials Science in Greenhouse Gas Mitigation Technology", A.V.G. Chizmeshya, Departmental Colloquium, Department of Physics and Astronomy, Host: R.B. Doak, Tempe, Arizona, November 7 (2002).

"Fundamental modeling of pre-carbonation treatment effects on serpentine and olivine feedstock", A.V.G. Chizmeshya, National Mineral Carbonation Working Group Meeting, U.S. Department of Energy, Office of Fossil Energy, Albany Research Center, Host: R. Walters, Albany, Oregon, September 10 (2002).

"Application of First principles Simulation to CO₂ Mineral Sequestration", A.V.G. Chizmeshya, 17th International Coal Conference, March 11-14, Clearwater, Florida (2002).

"Developing a Mechanistic Understanding of CO₂ Mineral Sequestration Reaction Processes," Michael J. McKelvy, Andrew V.G. Chizmeshya, Hamdallah Béarat, Renu Sharma, and R.W. Carpenter, presented at the 26th International Technical Conference on Coal Utilization & Fuel Systems, Host: B. Sakkestad, Clearwater, Florida, March 5-8, (2001).

"Developing a Mechanistic Understanding of Lamellar Hydroxide Mineral Carbonation Reaction Processes," Michael J. McKelvy, Andrew V.G. Chizmeshya, Hamdallah Béarat, Renu Sharma, R.W. Carpenter, Jason Diefenbacher, and George Wolf, an invited presentation at the U.S. Department of Energy Workshop on CO₂ Mineral Sequestration, Pittsburgh, Pennsylvania, August 8, 2001.

"Atomic-Level Imaging of CO₂ Disposal as a Carbonate Mineral: Optimizing Reaction Process Design," Michael J. McKelvy, Andrew V.G. Chizmeshya, Hamdallah Béarat, Renu Sharma, and R.W. Carpenter, presented at the University Coal Research Contractors Review Conference, Pittsburgh, Pennsylvania, June 5-6, 2001.

"Developing a Mechanistic Understanding of Lamellar Hydroxide Mineral Carbonation Reaction Processes to Reduce CO₂ Mineral Sequestration Process Cost," Michael J. McKelvy, Andrew V.G. Chizmeshya, Hamdallah Béarat, Renu Sharma, and R.W. Carpenter, an oral presentation at the First National Conference on Carbon Sequestration, Washington, D.C., May 14-17, 2001.

"Methods for Developing an Atomic-Level Understanding of Carbon Dioxide Mineral Sequestration Reaction Processes," Michael J. McKelvy, Andrew V.G. Chizmeshya, Hamdallah Béarat, Renu Sharma, and R.W. Carpenter, presented at the 2001 SME Meeting, Denver, Colorado, February 26-28, 2001.

"Atomic-Level Modeling of CO₂ Disposal as a Carbonate Mineral: A Synergetic Approach to Optimizing Reaction Process Design" A.V.G. Chizmeshya, R. Olsen and M.J. McKelvy, 21st Annual Combustion Research Conference, U.S. D.O.E. Office of Basic Energy Sciences, Host: Dr. W. Kirchoff, Chantilly, Virginia, June 2000.

"Atomic-Level Modeling of Mineral Carbonation Reaction Processes: Integrating Experiment with Theory" A.V.G. Chizmeshya, R. Olsen and M.J. McKelvy, University Coal Research Contractors Meeting, National Energy Technology Laboratory, Host: Phil Goldberg, Pittsburgh, PA, June 2000.

"Mg(OH)₂ Dehydroxylation: Implications for Enhancing CO₂ Mineral Sequestration Reaction Processes Process" M.J. McKelvy, R. Sharma, A.V.G. Chizmeshya, R.W. Carpenter and H. Bearat, *Proceedings of the 25th International Technical Conference on Coal Utilization and Fuel Systems, Clearwater, Florida, March 2000.*

"Developing and Atomic-Level Understanding to Enhance CO₂ Mineral Sequestration Reaction Processes Process via Materials and Reaction Engineering" M.J. McKelvy, R. Sharma, A.V.G. Chizmeshya, H. Bearat, R. Sharma and R.W. Carpenter, *Proc. 17th International Pittsburgh Coal Conference, Pittsburgh, Pennsylvania, September 2000.*

"Modern Modeling Strategies in Materials Science: Fact vs. Fantasy", A.V.G. Chizmeshya, *Adams' Research Group*, Department of Chem, Bio and Materials Engineering, Host: Prof. J. Adams, Arizona State University, Tempe, Arizona, January 22, (1999).

"Advanced Simulation and Modeling of Hydroxide Minerals: Dehydration and Carbonation" A.V.G. Chizmeshya, presented at the 4th Annual Carbon Dioxide Mineral Sequestration Forum, Host: Phil Goldberg, Arizona State University, December 9 (1999).

"Mg(OH)₂ Dehydroxylation: A Lamellar Nucleation and Growth Process" M.J. McKelvy, R. Sharma, A.V.G. Chizmeshya, R.W. Carpenter and K. Streib, *University Coal Researcher Contractors Review Meeting, Pittsburgh, Pennsylvania, July 1999.*

"Calculs *ab initio* de propriétés vibrationnelles et électroniques de la matière dense basés sur Density Functional Theory (DFT)", A. Chizmeshya, given in French at the École Normale Supérieure de Lyon, Host: Prof. P. Gillet, Lyon, France, March 12, (1998).

"Modélisation des structures et propriétés thermodynamiques de minéraux silicatés à haute pression: Application à la structure interne de la Terre", A. Chizmeshya, given in French at the Ecole Normale Supérieure de Lyon, Host: Prof. P. Gillet, Lyon, France, March 14 (1998).

"Thermoelastic Modeling of Complex Ceramics: A non-empirical density functional theory approach", A.V.G. Chizmeshya, G.H. Wolf and W.T. Petuskey, *Workshop on Multiscale Materials Prediction: Fundamentals and Industrial Applications*, MIT, Host: Prof. Sydney Yip, Boston, Massachusetts, September 14, (1997).

"Non-empirical Density Functional Description of the Thermoelastic Properties of Complex Ceramics", A.V.G. Chizmeshya, AFOSR Conference on Computer Aided Design of High-Temperature Materials, Host: Dr. A. Pechenik, Santa Fe, New Mexico, (August, 1997).

"*Ab Initio* Lattice Dynamics and Thermodynamics of Cubic Oxides, Sulfides and Perovskites", A. Chizmeshya, Department of Physics, Arizona State University, Host: Prof. O.F. Sankey, Tempe Arizona, April (1994).

"How to Calculate Thermoelastic Crystal Properties after you've Lost your CRAY Account!", A. Chizmeshya, T12 Theory Seminar, Los Alamos National Laboratory, Host: Prof. L. Pratt, Los Alamos, New Mexico, May (1994).

"First Principles Computer Simulation in Materials Science", A. Chizmeshya, Materials Research Group in High-pressure Synthesis, Host: Prof. P.F. McMillan, Arizona State University, Tempe, Arizona, October 12, (1993).

"A Simplified First Principles Approach to the Thermodynamics of Ionic Materials", A. Chizmeshya, Materials Research Group in High-pressure Synthesis, Host: Prof. P.F. McMillan, Arizona State University, Tempe, Arizona, December 3 (1993).

"A Local Density Functional Approach to the Treatment of Insulating Compounds and Ionic Materials", A. Chizmeshya, Department of Physics, Queen's University at Kingston, Host: Prof. E. Zaremba, Canada, September 23 (1993) .

"Electron Gas Theory of Ionic Solids: Application to Cubic Oxides and Silicate Perovskites", A. Chizmeshya, Department of Physics, University of Missouri at Rolla, Host: Prof. B. Hale, Rolla, Missouri, May (1999)

"The Adsorption of Inert Gases on Metal Surfaces", A. Chizmeshya, Center for Solid State Science, Arizona State University, Host: Prof. G.H. Wolf, Tempe, Arizona, September (1992).

PUBLICATIONS

Published Research Reports

"FUNDAMENTAL STUDIES OF ABOVE-GROUND AND GEOLOGIC MINERAL SEQUESTRATION REACTIONS", Andrew V. G. Chizmeshya; George H. Wolf; Hamdallah Bearat; R. Marzke, US DOE Argonne National Laboratory, 4F-01641(03) (OSTI ID: submitted), 36 pages, May (2010).

"Mineral sequestration reaction kinetics under above-ground and geologic settings", Andrew V. G. Chizmeshya ; George H. Wolf; Hamdallah Bearat; R. Marzke, US DOE Argonne National Laboratory, 4F-01641-02 (OSTI ID: submitted), 29 pages, May (2009).

"Fundamental studies of above-ground and geologic mineral sequestration reactions", Andrew V. G. Chizmeshya ; Hamdallah Bearat; George H. Wolf; R. Marzke, US DOE Argonne National Laboratory, 4F-01641-01 (OSTI ID: submitted), 39 pages, March (2008).

"A Novel Approach to Mineral Carbonation: Enhancing Carbonation While Avoiding Mineral Pretreatment Process Cost", Andrew V. G. Chizmeshya ; Michael J. McKelvy ; Kyle Squires ; Ray W. Carpenter ; Hamdallah Bearat, US DOE National Energy Technology Laboratory, FG26-04NT42124-03 (OSTI ID: 924162), 163 pages, June (2007).

"Enhancing the atomic-level understanding of CO₂ mineral sequestration mechanisms via advanced computational modeling", A.V.G. Chizmeshya ; M.J. McKelvy ; G.H. Wolf ; R.W. Carpenter ; D.A. Gormley ; J.R. Diefenbacher ; R. Marzke, US DOE National Energy Technology Laboratory, FG26-01NT41295-04 (OSTI ID: 883172), 109 pages, March (2006).

"Simultaneous mechanical and heat activation: A new route to enhance serpentine carbonation reactivity and lower CO₂ mineral sequestration process cost", M.J. McKelvy ; J. Diefenbacher ; R. Nunez ; R.W. Carpenter ; A.V.G. Chizmeshya, US DOE National Energy Technology Laboratory, FG26-02NT41546 (OSTI ID: 840464), 21 pages, January (2005).

"Understanding Olivine CO₂ mineral sequestration mechanisms at the atomic level: Optimizing reaction process design", M.J. McKelvy ; H. Bearat ; A.V.G. Chizmeshya ; R. Nunez ; R.W. Carpenter, US DOE National Energy Technology Laboratory, FG26-01NT41282 (OSTI ID: 822896), 17 pages, August (2003).

"Enhancing the atomic-level understanding of CO₂ mineral sequestration mechanisms via advanced computational modeling", A.V.G. Chizmeshya, US DOE National Energy Technology Laboratory, FG26-01NT41295-01 (OSTI ID: 883172), 29 pages, December (2002).

"Atomic-level modeling of CO₂ disposal as a carbonate mineral: A synergetic approach to optimizing reaction process design" A.V.G. Chizmeshya ; M.J. McKelvy ; J.B. Adams, US DOE FG26-99FT40580-01 (OSTI ID: 791496) 25 pages, November (2001).

"Atomic-level imaging of CO₂ disposal as a carbonate mineral: Optimizing reaction process design", M.J. McKelvy ; R. Sharma ; A.V.G. Chizmeshya ; H. Bearat ; R.W. Carpenter ; K. Streib, US DOE National Energy Technology Laboratory, FG26-98FT40112-01 (OSTI ID: 778329), 24 pages September (1999).

Pending Journal Publications (in preparation, review or press)

- P1. "Structural, Electronic and Optical properties of nano-structural BNC₃ alloys" A.V.G. Chizmeshya, submitted to Phys. Rev. B Nov 2016, (reviewed, revised and pending acceptance). [Support: NSF-SusChEM #1309090]
- P2. "First Principles Design of Silicon-compatible Si₂AlP alloy Absorber Materials: Optical Tuning via Nanostructure" A.V.G. Chizmeshya, (to be submitted to Chem. Mat.) [Support: NSF-SusChEM #1309090]
- P3. "Comparative Study of the Structural, Electronic and Thermoelastic Properties SiO₂ and Si(NH)₂ from First Principles" N. Masoumi, G.H. Wolf and A.V.G. Chizmeshya, (to be submitted to J. Phys. Chem. C)
- P4. "Beryllium Fluorocyanate: A novel covalently bonded ultra-light semiconductor based on earth abundant light elements", A.V.G. Chizmeshya, (to be submitted to Dalton Transactions)
- P5. "Direct Conversion of Carbon Dioxide to Molecular Oxygen at a Single-site Molybdenum Complex" R. Pal, A.V.G. Chizmeshya, T. Groy and R.J. Trovitch, (in preparation)
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FUNDING ACTIVITY

Most Recent Submissions

"Nitrogen Storage in the Mantle", National Science Foundation (EAR), **\$486,788** as **PI** with 2 others, January **2017** (pending).

"*Geomimicry: Catalysis in Water as a Universal Chemistry Paradigm*", National Science Foundation, Phase I Center for Chemical Innovation pre-proposal, **co-PI** with 5 others, Ian Gould (PI), September **2016** (pending)

"*Engineering Research Center for the Innovation for Carbon Capture, Utilization, and Storage (InFOCUS)*", National Science Foundation, **\$3,291,665** as **co-PI @ 5%** with 9 others, Klaus Lackner (PI), June **2016** (pending).

"*Water in Calcium Silicate Perovskite*" National Science Foundation, **\$489,318** as **co-PI @ 30%** with 2 others, Dan Shim (PI), July **2016** (declined).

"*Breaking the barrier between icy materials and silicates: The Geochemistry of Water World planets*" NASA Habitable Worlds Program, \$496,149, **co-PI @ 40%**, Dan Shim (PI), January **2016** (declined).

"*Computational Sciences Approaches to Self-Assembled Materials for Energy Conversion Applications*", US-DOE, **\$10,911,970**, **co-PI @ 15%** with 4 others, S. Goodnick (PI), April **2015** (declined).

"*MIP: Quantum Architecture of Designer Semiconductors*", National Science Foundation, **\$ 21,320,090** as **co-PI @ 2%** with 20 others, Y.-H. Zhang (PI), March **2015** (declined).

Current Awards

SusChEM: FRG: Molecular routes to new classes of polar/non-polar alloy semiconductors, **\$788,057** as **co-PI** 08/13-07/16, National Science Foundation (MPS-Physics)

"*Structural, energetic and optical properties of graphene oxide from first principles*", seed funding \$20K, **sole PI**, Northrop Grumman Aerospace

Past Awards

Sn-Containing Group-IV Semiconductors for Energy Applications in Photovoltaics and Thermoelectricity, **\$897,803 co-PI** 10/09-9/13, National Science Foundation

Fundamental Studies of Clay and Clay-Rich Mineral Reactions with H₂O-CO₂ fluids: Applications to Geological Sequestration, **PI** **\$554,000**, 04/2010-11/2012, Argonne National Laboratory, US Department of Energy.

Infrared and Terahertz Lasers on Si using Novel Group-IV Alloys, **co-PI** **\$2,600,000**, 7/1/2006–9/30/2011, Air Force Office of Scientific Research

Advance semiconductor materials for breakthrough photovoltaic applications, **co-PI** **\$893,020**, 01/08- 12/10, U.S. Department of Energy

Fundamental Studies of Above-Ground and Geologic and Mineral Sequestration Reactions, **PI** **\$528,438**, 6/07-10/09, U.S. Department of Energy / Argonne National Laboratory

Exploratory Study of Serpentine-based CO₂ Mineral Sequestration Reaction Optimization via Thermal Treatment, **PI** **\$96,210**, 2/08-9/09, ORICA Inc. (Australia)

Southwest Regional Partnership on CO₂ Geologic Sequestration, **PI** **\$14,210/year**, 9/07-8/10, U.S. Department of Energy/ National Energy Technology Laboratory

Project Pathways: Opening Routes To Math And Science Success For All Students, co-PI
\$2,390,750, 9/15/2004-8/31/2009, National Science Foundation

UHV-CVD hybrid deposition system for semiconductor synthesis, co-PI
\$250,000, 6/07- 5/09, AFOSR Defense University Research Instrumentation Program (DURIP)

Hybrid substrates for low cost solid-state lighting generation and solar energy applications, co-PI
\$270,000, 5/1/07 - 4/31/08, Science Foundation Arizona

IMR: Acquisition of a Multi-purpose High Resolution X-ray Diffraction User Facility for Materials Research and Education, co-PI
\$245,000 11/1/05 to 10/31/07 NSF-DMR

ASU-Voltaix Seed Project in Fundamental Computational Studies of Si-Ge-hydrides, **PI**
\$2,500 12/23/06 to 3/1/07 Voltaix Corporation

In Situ Investigations of Mechanisms than Govern CO₂ Mineral Sequestration Reaction Processes, co-PI
\$334,676 6/1/04 to 5/31/06 DOE/NETL/ANL

A Novel Approach to Mineral Carbonation: Enhancing Carbonation while Avoiding Mineral Pretreatment Process Cost, co-PI
\$430,482 6/22/04 to 6/21/06 DOE/ National Academy of Sciences

In Situ Real-time Atomic/Nanoscale Materials Synthesis, Characterization and Modeling for Undergraduate Education, co-PI
\$100,000 7/1/04 to 6/30/06 NSF/NUE

Enhancing the Atomic-Level Understanding of CO₂ Mineral Sequestration Mechanisms via Computational Modeling, **PI**
\$195,717 9/20/01 to 9/19/05 DOE/NETL

The Fundamental Studies On Icosahedral Borides For Beta Cell Applications, co-PI
\$286,956 Qynergy Corp. 5/16/2004-8/30/2005

Mechanistic And Computational Study Of Cinnabar Phase Transformation: Applications And Implications To The Preservation Of This Pigment, co-PI
\$77,382 10/15/02-10/15/04 U.S. Department of the Interior

MRI: Acquisition Of A Field-Emission, Controlled Temperature Environmental Scanning Electron Microscope For Multidisciplinary Research, co-PI
\$713,135 NSF-MRI

Simultaneous Mechanical And Heat Activation: A New Route To Enhance Serpentine Carbonation Reactivity And Lower CO₂ Mineral Sequestration, co-PI
\$71,896 9/15/01-9/14/03, U.S. Department of Energy, NETL

Atomic Level Modeling of CO₂ Disposal as a Carbonate Mineral: A Synergetic Approach to Optimizing Reaction Design, **PI**
\$64,093 8/31/00-8/31/02, U.S. Department of Energy.

Patent and Intellectual Property Activity

Continuation Patent: Silicon-Germanium hydrides and methods for making and using same Inventors: John Kouvetakis, Cole J. Ritter, Changwu Hu, Ignatius S.T. Tsong and Andrew V.G. Chizmeshya USPTO #8518360 B2, Assignee: Arizona Board Of Regents, Issued August 27 (2013)

Silicon-Germanium hydrides and methods for making and using same Inventors: John Kouvetakis, Cole J. Ritter, Changwu Hu, Ignatius S.T. Tsong and Andrew V.G. Chizmeshya USPTO #8216537, PCP WO2007/062056, Assignee: Arizona Board Of Regents, Issued July 10 (2012)

High-Temperature Treatment of Hydrous Minerals Inventors: Andrew V.G. Chizmeshya and Geoffrey F. Brent, EPO

#2477945 A2, WO2011035047, Assignee: Arizona Board Of Regents, Issued July 25 (2012)

High-temperature treatment of hydrous minerals Andrew V.G. Chizmeshya and Geoffrey F. Brent, Andrew V. Granted Innovation Pat. (Aust.), (2011), 35pp. CODEN: AUXXBL AU 2010101031.

High-temperature flash treatment of CO sequestration feedstock minerals Chizmeshya, Andrew V. (The Arizona Board of Regents, a Body Corporate Acting on behalf of Arizona State University, USA). PCT Int. Appl. pending (submitted, Jan 2009)

Novel silicon-germanium hydrides which give Ge-Si films with low dislocation densities and surface roughness and methods for synthesis and use in deposition methods. Kouvetakis, John; Ritter, Cole J., III; Hu, Changwu; Tsong, Ignatius S. T.; Chizmeshya, Andrew. (The Arizona Board of Regents, a Body Corporate Acting on behalf of Arizona State University, USA). PCT Int. Appl. (2007), WO 2006-US45091.

Microreactor with controllable pressure and temperature for in situ material investigations. McKelvy, Michael J.; Diefenbacher, Jason; Wolf, George H.; Chizmeshya, Andrew V.. (Arizona Board Regents, a Body Corporate of the State of Arizona Acting for and on Behalf of Arizona State University, USA). PCT Int. Appl. (2006), WO2005-US23426.

Non-monetary Awards

"Fundamental Studies of Clay and Clay-rich mineral reactions with H₂O-CO₂ fluids: Applications to Geological Carbon Sequestration," A.V.G. Chizmeshya. U.S. Department of Energy/Argonne National Lab, 7/18/12 to 7/22/12. Beamtime award # GUP-27851 (2012).

"Fundamental Studies of Clay and Clay-rich mineral reactions with H₂O-CO₂ fluids: Applications to Geological Carbon Sequestration," A.V.G. Chizmeshya. U.S. Department of Energy/Argonne National Lab, 8/3/11 to 8/7/11. Beamtime award # GUP-23801 (2011).

"Microreactor Beamline Development for Low Energy Focused Beam Applications", J.R. Diefenbacher and A.V.G. Chizmeshya. U.S. Department of Energy/Argonne National Lab, 7/21/11 to 7/25/11. Beamtime award # GUP-23123 (2011).

70,000 SU Allocation Award – ASU Fulton HPCI 9/1/10-9/2/12.

"Fundamental Studies of Clay and Clay-rich mineral reactions with H₂O-CO₂ fluids: Applications to Geological Carbon Sequestration," A.V.G. Chizmeshya. U.S. Department of Energy/Argonne National Lab, 7/8/10 to 7/7/11. Beamtime award # GUP-22304 (2010).

"Fundamental Studies of Clay and Clay-rich mineral reactions with H₂O-CO₂ fluids: Applications to Geological Carbon Sequestration," A.V.G. Chizmeshya. U.S. Department of Energy/Argonne National Lab, 2/25/10 to 3/5/10. Beamtime award # GUP-22801 (2010).

"In Situ Mechanistic Observations of Serpentine Mineral Carbonation Reaction Processes: Facilitating the Engineering of Lower Cost Carbon Dioxide Sequestration Options," A.V.G. Chizmeshya, G. Wolf, H. Bearat. U.S. Department of Energy/Argonne National Lab, 6/10/09 to 6/14/09. Beamtime award # GUP-11986 (2009).

"In Situ Mechanistic Observations of Serpentine Mineral Carbonation Reaction Processes: Facilitating the Engineering of Lower Cost Carbon Dioxide Sequestration Options," A.V.G. Chizmeshya, G. Wolf, H. Bearat. U.S. Department of Energy/Argonne National Lab, 11/5/08 to 11/9/08. Beamtime award # GUP10601 (2008).

"In Situ Mechanistic Observations of Serpentine Mineral Carbonation Reaction Processes: Facilitating the Engineering of Lower Cost Carbon Dioxide Sequestration Options," A.V.G. Chizmeshya, G. Wolf, H. Bearat. U.S. Department of Energy/Argonne National Lab, 2/27/08 to 3/03/08. Beamtime award # G009123 (2008).

50,000 SU Allocation Award – ASU Fulton HPCI 12/22/06-12/21/07.

Provisional Patent (ASU #M2-084) "Externally Controlled Chemical Microreactor for Reaction Investigation Under Supercritical and Subcritical Conditions", co-inventor (2003).

32,000 SU Allocation Award #MP3020001P - Pittsburgh Supercomputer Center 5/31/03-6/1/04

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