Curriculum Vitae

Evangelos Miliordos

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Education

April 2006 – March 2010	National and Kapodistrian University, Athens, Greece Department of Chemistry *Advisor*: Prof. Aristides Mavridis Ph.D. in Physical Chemistry granted May 2010
September 2003 – March 2006	National and Kapodistrian University, Athens, Greece Department of Chemistry *Advisor*: Prof. Aristides Mavridis M.Sc. in Physical Chemistry granted March 2006
September 1999 – September 2003	National and Kapodistrian University, Athens, Greece Department of Chemistry B.Sc. in Chemistry granted December 2003

Professional Employment

April 2026 – May 2026	***Visiting Professor*** Department of Chemistry and Applied Biosciences Swiss Federal Institute of Technology in Zurich (Eidgenössische Technische Hochschule, ETH) Zürich, Switzerland
January 2024 – today	***Co-director of CM^4*** Center for Multiscale Modeling of Materials and Molecules (CM^4) College of Sciences and Mathematics Auburn University Auburn, Alabama, USA
August 2020 – today	***Chair of the Physical Chemistry Division*** Department of Chemistry and Biochemistry Auburn University Auburn, Alabama, USA

October 2022 – today
James E. Land Associate Professor
Department of Chemistry and Biochemistry
Auburn University
Auburn, Alabama, USA

September 2022 – December 2022
Visiting Professor
Department of Chemistry and Applied Biosciences
Swiss Federal Institute of Technology in Zurich
(Eidgenössische Technische Hochschule, ETH)
Zürich, Switzerland

October 2020 – September 2022
James E. Land Assistant Professor
Department of Chemistry and Biochemistry
Auburn University
Auburn, Alabama, USA

June 2016 – September 2020
Assistant Professor
Department of Chemistry and Biochemistry
Auburn University
Auburn, Alabama, USA

June 2015 – June 2016
Postdoctoral Fellow
Catalysis Center for Energy Innovation (EFRC)
University of Delaware
Newark, Delaware, USA
Research advisor: D. G. Vlachos

September 2012 – June 2015
Postdoctoral Fellow
Physical Sciences Division
Pacific Northwest National Laboratory
Richland, Washington, USA
Research advisor: S. S. Xantheas

May 2010 – June 2012
Postdoctoral Fellow
Department of Chemistry
Michigan State University
East Lansing, Michigan, USA
Research advisor: K. L. C. Hunt

May 2008 – May 2009
Military Service
Greek army

September 2006 – June 2007
Graduate Teaching Assistant
Department of Chemistry
National and Kapodistrian University
Athens, Greece

Fellowships

Graduate fellowship, three-year fellowship from the Hellenic National Scholarships Foundation (I.K.Y.) for graduate studies (academic years 2006-2008, 2009-2010).

Marie Curie fellowship, Professor Petr Čársky's laboratory, Heyrovský Institute, Prague, Czech Republic (July – October 2004).

Awards and Distinctions – Professional Recognition

Undergraduate awards, awarded three times by the Hellenic National Scholarships Foundation (I.K.Y.) for undergraduate studies performance (academic years 1999, 2001, 2002)

Outstanding performance award, Fundamental and Computational Sciences Directorate, Pacific Northwest National Laboratory (December 2013)

James E. Land endowment, Auburn University (October 2020 – September 2023)

OpenEye Outstanding Junior Faculty Award in Computational Chemistry, American Chemical Society (April 2021)

Dean's Research Award, College of Sciences and Mathematics, Auburn University (April 2022)

Young Investigator Scholar Award, College of Sciences and Mathematics, Auburn University (March 2025)

Membership in Professional Societies

American Chemical Society (ACS), 2013 – present ACS member ID: 30134004
American Physical Society (APS), 2017 – present APS member ID: 61249631
American Institute of Chemical Engineers (AICHE), 2020 – 2024 AICHE member ID: 009904802549
Association of Greek Chemists, 2003 – 2008

Teaching Experience

Auburn University: *CHEM 1030* General Chemistry I (undergraduate level)
CHEM 1117 General Chemistry I – Honors (undergraduate level)
CHEM 4070 Physical Chemistry I (thermodynamics/kinetics; undergraduate level)
CHEM 4071 Physical Chemistry I Lab (computational chemistry lab)
CHEM 4080 Physical Chemistry II (quantum mechanics; undergraduate level)
CHEM 5280/6280 Computational Chemistry (undergraduate/graduate level)
CHEM 7300 Advanced Physical Chemistry (graduate level)
CHEM 7330 Chemical kinetics (graduate level)
CHEM 3160 Survey of Physical Chemistry (undergraduate level)

Students Recruiting Activities

2018 Talented Academic Leaders Outstanding National Scholars (TALONS), Auburn, Alabama, USA (January 26)

2018 Southeastern Undergraduate Research Conference, Oxford, Mississippi, USA (February 2-3)

2021 SouthEast Regional Meeting of the American Chemical Society (SERMACS), Birmingham, Alabama, USA (November 10-13)

2024 10th Symposium of Electronic Structure and molecular Dynamics (SEEDMOL), Pirenopolis, Goias, Brazil (November 4-8)

2025 University of Brasilia, Brasilia, Federal District, Brazil (December 9)

Students and Post-doctoral Researchers Mentored

High-School students:

Daniel Pacheco (Alabama School of Math and Science, 2024-2025)

Undergraduate students:

Jacob Mayhugh (2016-2017)
Holden Paz (2018-2019)
Marissa Miltersen (2020)
Isabel Franklin (2021)
Pallavi Nair (2021)
Zachary Jordan (2021)
Zhongyuan Lu (2021-2022)
Jared Stinson (2021)
Brody Quebedeaux (2021-2023)
Debora Vasconcelos (2023-2025)
Charlie Greenleaf (2025-2026)
Samuel Lenz (2025-2026)
Sydney Risch (2025-present)
Emma Shea (2025-present)

Graduate students:

Isuru Ariyarathna (2016-2021)
Shahriar Khan (2016-2021)
Holden Paz (2020-2022)
Emily Claveau (2018-2023)
Benjamin Jackson (2018-2023)
Safaa Sader (2019-2023)
Eslam Fathy Mohamed Abdelazim (2022-2024)
Andrei Evdokimov (2023-present)
Alexandros Androutsopoulos (2023-present)
Taylor Gregory (2024-present)
Joseph Olaniyan (2024-present)

Post-doctoral Researchers:

Nuno Almeida (2017-2019)

Achievements of Graduate and High-school (*) Students

Isuru Ariyarathna: poster award at SETCA 2018, poster award at "This is research" student symposium (Auburn, 2018), Outstanding Graduate Student Award (Auburn, 2019), Dow fellowship (Auburn, 2019), Dean's Research Award (Auburn, 2019), Outstanding International Graduate Student Award (Auburn, 2021), Harry Meriwether fellowship (Auburn, 2020-2021), NOBCChe Collaborative Abstract (May 2021), Chemical Computing Group Excellence Award from the Computers in Chemistry Division of the American Chemical Society (2021), Distinguished Dissertation Award (Auburn, 2022)

Shahriar Khan: Graduate Research and Travel Fellowship (Auburn, 2020), Graduate Student Council (GSC) Travel Fellowship (Local ACS Section, 2020), Outstanding International Graduate Student Award (Auburn 2021), Internship at Los Alamos National Laboratory (May-August 2021)

Benjamin Jackson: Newman award (Auburn, 2020), Dean's Research Award (Auburn, 2022), DoE Science Graduate Student Research Fellowship (PNNL, June 13 – September 13, 2022, first time across STEM in Auburn)

Emily Claveau: Dow Fellowship (Auburn, 2022), COSAM Graduate Student Travel Award (Auburn, 2022)

Safaa Sader: Researcher Development Grants (Royal Society of Chemistry, January 2023)

Alexandros Androutsopoulos: Internship at Los Alamos National Laboratory (June-August 2024 and June-August 2025)

Andrei Evdokimov: Internship at Oak Ridge National Laboratory (May-July 2025), poster award at SETCA 2025, Dow fellowship (Auburn, 2026)

Daniel Pacheco*: Third place at the Mobile Regional Science & Engineering Fair (MRSEF) (February 28, 2025), advanced to the National Level Competition at the Alabama Science and Engineering Fair (ASEF) (April 5, 2025)

Reviewing Activities

Journals: The Journal of Chemical Physics, Chemical Physics, Journal of Quantitative Spectroscopy and Ratiative Transfer, Chemical Physics Letters, Journal of Physical Chemistry, The Journal of Physical Chemistry Letters, Computational Material Science, Computational and Theoretical Chemistry, International Journal of Quantum Chemistry, ACS Omega, Symmetry, Journal of American Chemical Society, Computational and Structural Biotechnology Journal, Chemical Communications, Journal of Fluorine Chemistry, Inorganic Chemistry, Journal of Molecular Structure, ChemPlusChem, Physical Chemistry Chemical Physics, Applied Physics Letters, National Science Review, Chemical Science, Physica E, Physica B, Journal of Chemical Education, Catalysis Science and Technology, Monthly Notices of the Royal Astronomical Society, Journal of Physical Chemistry Letters, Inorganic and Nano-Metal Chemistry, ACS Organic & Inorganic Au, Chemistry: A European Journal, Organometallics, Journal of Solid State Chemistry, Transition Metal Chemistry, Journal of Molecular Modeling, Chinese Journal of Structural Chemistry, Dalton Transactions, Journal of Computational and Theoretical Chemistry, Nature Communications, Theoretical Chemistry Accounts, Discover Chemistry, Review of Materials Research

Agencies: Department of Energy (DOE/BES), American Chemical Society (ACS-PRF and ACS-COMP), National Science Foundation (regular, center, and GRFP proposals, ad-hoc reviewer and panelist), Auburn University (internal proposals)

Institutions: Evaluation of the physical chemistry program of the chemistry department at the National and Kapodistrian University of Athens, Greece (2024)

Outreach Activities

2016 ΦΛΥ sorority, Auburn University, Auburn, Alabama, USA (October 18)

2017 Panelist at "Navigating the real world with a PhD", an event organized by the graduate students association, Auburn University, Auburn, Alabama, USA (November 29)

2018 Summer Science Institute organized by the College of Sciences and Mathematics, Auburn University, Auburn, Alabama, USA (June 11)

2018 Computational Chemistry seminar for non-computational chemists, Auburn University, Auburn, Alabama, USA (November 14)

2021 Summer Science Institute organized by the College of Sciences and Mathematics, Auburn University, Auburn, Alabama, USA (June 10)

2021 Organized the symposium “Theoretical chemistry: Method development and applications” in the SouthEast Regional Meeting of the American Chemical Society (SERMACS, Birmingham, Alabama, USA, November 10-13)

2022 Judge for the “This is Research” Symposium, Auburn (March 29)

2022 Summer Science Institute organized by the College of Sciences and Mathematics, Auburn University, Auburn, Alabama, USA (June 9)

2023 Summer Science Institute organized by the College of Sciences and Mathematics, Auburn University, Auburn, Alabama, USA (June 5)

2024 Summer Science Institute organized by the College of Sciences and Mathematics, Auburn University, Auburn, Alabama, USA (June 4)

2025 Summer Science Institute organized by the College of Sciences and Mathematics, Auburn University, Auburn, Alabama, USA (June 3)

2025 “Chemical bonding theories confuse you? They confuse me too!”, Tuskegee University, Tuskegee, Alabama, USA (February 21)

2026 “Puzzled with chemical bonding? Let’s put the jigsaw pieces together”, Auburn University, Auburn, Alabama, USA (March-April) – IRB approved survey on undergraduate general chemistry education

2026 “Science and God” seminar series in collaboration with the Baptist Campus Ministries organization

Professional Service

2020-now Director of the Physical Chemistry division (Department of Chemistry and Biochemistry, Auburn University)

2024-now Co-director of CM^4 (Center for Multiscale Modeling of Materials and Molecules)

2017 Member of the hiring committee for an Assistant Professor in Atomic, Molecular, and Optical Physics (Department of Physics, Auburn University)

2020 Member of the hiring committee for an Assistant Professor in Computational Chemistry (Department of Chemistry and Biochemistry, Auburn University)

2021-2022 Member of the hiring committee for the Dean of the College of Sciences and Mathematics, Auburn University

2022-2023 Guest-Editor for Molecules (special Issue with the theme: "Insights in Chemistry and Spectroscopy of Excited Electronic States From Theoretical Calculations")
2024 Chair of the hiring committee for an Assistant Professor in Computational Chemistry (Department of Chemistry and Biochemistry, Auburn University)
2024-2026 Vice-Chair for the Gordon Research Conference (GRC) meeting on Molecular and Ionic Clusters
2026-2028 Chair for the Gordon Research Conference (GRC) meeting on Molecular and Ionic Clusters

Citation Index

Google Scholar:	Total of 2761 citations (as of April 30, 2026)	Hirsch index: 29
Web of Science	Total of 2169 citations (as of April 30, 2026)	Hirsch index: 26

Invited Talks at Scientific Institutions

2012 Michigan State University, East Lansing, Michigan, USA; Physical Chemistry Seminar (April 24)
2012 Pacific Northwest National Laboratory, Richland, Washington, USA (May 7)
2012 National Hellenic Research Foundation, Athens, Greece (July 3)
2013 Michigan State University, East Lansing, Michigan, USA; Physical Chemistry Seminar (May 6)
2014 Pacific Northwest National Laboratory, Richland, Washington, USA (April 16)
2015 Johns Hopkins University, Baltimore, Maryland, USA (November 13)
2016 Auburn University, Auburn, Alabama, USA (February 23)
2016 National and Kapodistrian University of Athens, Athens, Greece (June 30)
2016 Energy Cluster Symposium, Auburn University, Auburn, Alabama, USA (August 8)
2016 Physical Chemistry Seminar, Auburn University, Auburn, Alabama, USA (August 30)
2016 Auburn University, Department of Physics, Auburn, Alabama, USA (September 9)
2017 Physical Chemistry Seminar, Auburn University, Auburn, Alabama, USA (February 7)
2017 Physical Chemistry Seminar, University of Tennessee, Knoxville, Tennessee, USA (May 12)
2020 Johns Hopkins University, Baltimore, Maryland, USA (February 4)
2020 Temple University, Philadelphia, Pennsylvania, USA (February 5)
2020 University of Delaware, Newark, Delaware, USA (February 7)
2021 University of Alabama (remote visit), USA (February 11)
2021 University of Massachusetts (remote visit), USA (April 15)
2021 Georgia State University (remote visit), USA (October 14)
2022 National and Kapodistrian University of Athens, Athens, Greece (September 13)
2022 The National Hellenic Research Foundation, Athens, Greece (remotely, October 13)
2022 Max-Planck-Institut für Kernphysik, Heidelberg, Germany (November 9)
2022 Swiss Federal Institute of Technology / Eidgenössische Technische Hochschule (ETH) Zürich, Switzerland (December 6)
2023 University of Akron, Akron, Ohio, USA (February 21)
2023 University of Pittsburgh, Pittsburgh, Pennsylvania, USA (February 24)
2024 University of Brasilia, Brasilia, Federal District, Brazil (October 30)
2025 National and Kapodistrian University of Athens, Athens, Greece (July 8)
2025 University of Brasilia, Brasilia, Federal District, Brazil (December 9)
2026 University of Innsbruck, Innsbruck, Austria (May 6)

2026 Swiss Federal Institute of Technology / Eidgenössische Technische Hochschule (ETH) Zürich, Switzerland (May 22)

Invited Talks in Scientific Conferences/Meetings

2013 Telluride Science Research Center, "Intermolecular Interactions: New challenges for ab initio Theory", Telluride, Colorado, USA (July 15 – 19)

2014 Collaborative Workshop in Chemistry at the Interfaces, University of California at Irvine, Laguna Beach, California, USA (January 22 – 23)

2016 251st American Chemical Society meeting, San Diego, California, USA (March 13 – 17)

2017 South East Theoretical Chemistry Association meeting, Oxford, Mississippi, USA (May 18 – 20)

2017 Mid-West Theoretical Chemistry Conference, East Lansing, Michigan, USA (June 1 – 3)

2017 Computational Chemistry / Computational Modeling meeting at Environmental Laboratory, US Army Corps Engineering Research and Development Center, Vicksburg, Mississippi, USA (September 12)

2017 1st North-West Theoretical Chemistry Conference, Richland, Washington, USA (October 26 – 28)

2018 255th American Chemical Society meeting, New Orleans, Louisiana, USA (March 18 – 22)

2018 South East Theoretical Chemistry Association meeting, Baton Rouge, Louisiana, USA (May 18 – 19)

2018 International Conference of Chemical Bonding, Kauai, Hawaii, USA (July 13 – 17)

2019 *Session Chair*, South-East Theoretical Chemistry Association meeting, Knoxville, Tennessee, USA (May 16 – 18)

2021 American Chemical Society Spring 2021 virtual meeting (April 5 – 30)

2021 American Chemical Society Fall 2021 virtual meeting (August 22 – 26)

2022 Invited communication at World Association of Theoretical and Computational Chemists (WATOC 2020), Vancouver, Canada (July 3-8)

2024 Session Chair, Molecular and Ionic Clusters Gordon Conference, Ventura, California, USA (February 4-9)

2024 23rd Panhellenic Chemistry Conference, Athens, Greece (September 25-28)

2024 10th Symposium of Electronic Structure and molecular Dynamics (SEEDMOL), Pirenopolis, Goias, Brazil (November 4-8)

2024 5th International Caparica Christmas Conference on Translational Chemistry (IC3TC), Lisbon, Portugal (December 8-12)

Participation and Contributed Talks in Scientific Conferences/Meetings

2003 *Participant*, 8th European Workshop on Quantum Systems in Chemistry and Physics, Spetses, Greece (August 30 – September 4)

2004 *Poster presentation*, Molecular Quantum Mechanics: The No Nonsense Path to Progress, St. John's College, Cambridge University, England, UK (July 24 – 29)

2004 *Poster presentation*, 3rd Central European Symposium on Theoretical Chemistry, Tihany, Balaton, Hungary (September 30 – October 3)

2006 *Poster presentation*, 7th International Conference of Computational Methods in Sciences and Engineering, Chania, Crete, Greece (October 30 – November 1)

2009 *Contributed Talk*, 1st Conference of the Graduate Students of the National and Kapodistrian University of Athens, Athens, Greece (March 27 – 28)

2009 *Attendance*, 18th Symposium of the Hellenic Nuclear Physics Society, Athens, Greece (May 29 – 30)

2011 *Poster presentation*, DFT 2011, Athens, Greece (August 29 – September 2)

2012 *Contributed Talk*, 2012 Midwest Theoretical Chemistry Conference, Madison, Wisconsin, USA (June 7 – 9)

2013 *Contributed Talk*, 246th American Chemical Society meeting, Indianapolis, Indiana, USA (September 8 – 12)

2014 *Poster presentation*, 2014 Midwest Theoretical Chemistry Conference, Evanston, Illinois, USA (June 15 – 17)

2014 *Poster presentation*, Telluride Science Research Center, American Conference on Theoretical Chemistry, Telluride, Colorado, USA (July 20 – 24)

2014 *Contributed Talk*, PNNL Post-doc Symposium, Richland, Washington, USA (July 30)

2015 *Attendance*, 2015 Research Review of the Center for Catalysis, Science and Technology, Newark, Delaware, USA (October 7 – 8)

2016 *Poster presentation*, 2016 Catalysis Center for Energy Innovation Spring Symposium, Newark, Delaware, USA (April 10 – 11)

2018 *Contributed Talk*, International Symposium on Molecular Spectroscopy, Urbana-Champaign, Illinois, USA (June 18 – 22)

2018 *Contributed Talk*, Mid-West Theoretical Chemistry Conference, Chicago, Illinois, USA (June 21 – 23)

2018 *Contributed Talk*, Southeastern Regional Meeting of the American Chemical Society (SERMACS), Augusta, Georgia, USA (October 31 – November 3)

2019 *Contributed Talk*, Gordon Research Conference (GRC), Gaseous Ions: Structures, Energetics and Reactions, Ventura, California, USA (February 17 – 22). *Abstract selected for a Hot Topic talk*

2019 *Attendance*, Machine Learning in Science and Engineering, Atlanta, Georgia, USA (June 10 – 12)

2019 *Contributed Talk*, American Chemical Society National meeting, San Diego, California, USA (August 25 – 29)

2020 *Contributed talk and poster presentation*, American Institute of Chemical Engineers National conference, virtual meeting (November 16-20)

2021 *Contributed talk*, Pacifichem conference (symposium in honor of Keiji Morokuma), virtual meeting (December 16-21)

2022 *Contributed Talk*, 61st Sanibel Symposium, St Simons Island, Georgia, USA (February 13 – 18). *Abstract selected for a Hot Topic presentation*

2022 *Contributed Talk*, American Chemical Society Spring 2022 National meeting, San Diego, California, USA (March 20 – 24). *Symposium in honor of John Stanton*

2022 Poster presentation, Gordon Research Conference (GRC), Catalysis, New London, New Hampshire, USA (June 19 – 24)

2022 Contributed Talk, Dynamics of Electrons in Atomic and Molecular Nanoclusters, Erice, Italy (August 25 – 31). *Abstract selected for a Hot Topic talk*

2023 Poster presentation, Gordon Research Conference (GRC), Inorganic Reaction Mechanisms, Galveston, Texas, USA (March 5 – 10)

2023 NSF EPSCoR Workshop on Quantum Computing, Information, Science, and Engineering, Alexandria, Virginia, USA (March 23-24)

2023 Poster presentation, Heavy Element Chemistry Principal Investigators' Meeting, Washington DC, USA (April 23-25)

2023 Contributed Talk, International Meeting on Atomic and Molecular Physics and Chemistry (IMAMPC), Innsbruck, Austria (June 11-14). *Abstract selected for a Hot Topic talk*

2024 Contributed Talk, 75th Southeastern Regional Meeting of the American Chemical Society, Atlanta, Georgia, USA (October 23 – 26)

2025 American Chemical Society Fall meeting, Washington, D.C., USA (August 17 – 21)

2026 American Society of Mass Spectrometry meeting, San Diego, California, USA (May 31 – June 4)

2026 American Chemical Society Spring meeting, Atlanta, Georgia, USA (March 22 – 26)

2026 Poster presentation, Inorganic Chemistry Gordon Research Conference, Newport, Rhode Island, USA (May 31 – June 5)

2026 Poster presentation, Gordon Research Conference (GRC), Molecular and Ionic Clusters, Barga, Lucca, Italy (April 19 – 24)

Poster Presentations of graduate / undergraduate (*) / high-school (**) students

2017 Shahriar Khan, South East Theoretical Chemistry Association Meeting, Oxford, Mississippi, USA (May 18 – 20)

2017 Isuru Ariyarathna, South East Theoretical Chemistry Association Meeting, Oxford, Mississippi, USA (May 18 – 20)

2017 Isuru Ariyarathna, This is Research (student symposium), Auburn, Alabama, USA

2018 Shahriar Khan, 255th American Chemical Society National Meeting, New Orleans, Louisiana, USA (March 18 – 22)

2018 Shahriar Khan, South East Theoretical Chemistry Association Meeting, Baton Rouge, Louisiana, USA (May 18 – 19)

2018 Shahriar Khan, 70th Southeastern Regional Meeting of American Chemical Society, Augusta, Georgia, USA (October 31 – November 3)

2018* Jacob Mayhugh, 70th Southeastern Regional Meeting of American Chemical Society, Augusta, Georgia, USA (October 31 – November 3)

2018 Isuru Ariyarathna, 255th American Chemical Society National Meeting, New Orleans, Louisiana, USA (March 18 – 22)

2018 Isuru Ariyarathna, South East Theoretical Chemistry Association Meeting, Baton Rouge, Louisiana, USA (May 18 – 19)

2018 Isuru Ariyarathna, 70th Southeastern Regional Meeting of American Chemical Society, Augusta, Georgia, USA (October 31 – November 3)

2018 Isuru Ariyarathna, This is Research (student symposium), Auburn, Alabama, USA

2019 Shahriar Khan, South East Theoretical Chemistry Association Meeting, Knoxville, Tennessee, USA (May 16 – 18)

2019 Isuru Ariyarathna, South East Theoretical Chemistry Association Meeting, Knoxville, Tennessee, USA (May 16 – 18)

2019 Emily Claveau, South East Theoretical Chemistry Association Meeting, Knoxville, Tennessee, USA (May 16 – 18)

2019 Benjamin Jackson, South East Theoretical Chemistry Association Meeting, Knoxville, Tennessee, USA (May 16 – 18)

2019 Isuru Ariyarathna, This is Research (student symposium), Auburn, Alabama, USA

2019 Isuru Ariyarathna, 59th Sanibel Symposium, St. Simons Island, Georgia, USA (February 17 – 22)

2020 Emily Claveau, American Institute of Chemical Engineers virtual meeting

2020 Benjamin Jackson, American Institute of Chemical Engineers virtual meeting

2020 Isuru Ariyarathna, American Institute of Chemical Engineers virtual meeting

2021 Emily Claveau, American Chemical Society Spring 2021 virtual meeting (April 5 – 30)

2021 Benjamin Jackson, American Chemical Society Spring 2021 virtual meeting (April 5 – 30)

2021 Isuru Ariyarathna, American Chemical Society Spring 2021 virtual meeting (April 5 – 30)

2021 Benjamin Jackson, SouthEast Regional Meeting of the American Chemical Society (SERMACS), Birmingham, Alabama, USA (November 10-13)

2021 Safaa Sader, SouthEast Regional Meeting of the American Chemical Society (SERMACS), Birmingham, Alabama, USA (November 10-13)

2022 Safaa Sader, South East Theoretical Chemistry Association Meeting, Atlanta, Georgia, USA (May 19 – 21)

2022 Benjamin Jackson, South East Theoretical Chemistry Association Meeting, Atlanta, Georgia, USA (May 19 – 21)

2022 Emily Claveau, South East Theoretical Chemistry Association Meeting, Atlanta, Georgia, USA (May 19 – 21)

2022 Emily Claveau, American Chemical Society Spring 2022 National Meeting, San Diego, California, USA (March 20 – 24)

2022 Benjamin Jackson, World Association of Theoretical and Computational Chemists (WATOC 2020), Vancouver, Canada (July 3-8)

2022 Benjamin Jackson, Auburn Research Student Symposium, Auburn, Alabama, USA (March 28)

2024 Andrei Evdokimov, ACS Local Section Research Symposium, Troy, Alabama, USA (February 23)

2024 Andrei Evdokimov, 63rd Sanibel Symposium, St. Augustine Beach, Florida, USA (February 25 – March 1)

2024 Andrei Evdokimov, American Chemical Society Fall 2024 National Meeting, Denver, Colorado, USA (August 17-22)

2024 Andrei Evdokimov, 75th Southeastern Regional Meeting of the American Chemical Society, Atlanta, Georgia, USA (October 23-26)

2024* Debora Vasconcelos, 75th Southeastern Regional Meeting of the American Chemical Society, Atlanta, Georgia, USA (October 23-26)

2024 Alexandros Androutsopoulos, 75th Southeastern Regional Meeting of the American Chemical Society, Atlanta, Georgia, USA (October 23-26)

2025 Taylor Gregory, 2nd Symposium of the local ACS section, Columbus, Georgia, USA (March 1)

2025 Joseph Olaniyan, 2nd Symposium of the local ACS section, Columbus, Georgia, USA (March 1)

2025 Alexandros Androutsopoulos, 2nd Symposium of the local ACS section, Columbus, Georgia, USA (March 1)

2025 Andrei Evdokimov, 2nd Symposium of the local ACS section, Columbus, Georgia, USA (March 1)

2025** Daniel Pacheco, Mobile Regional Science & Engineering Fair (MRSEF), Mobile, Alabama, USA (February 28)

2025** Daniel Pacheco, Alabama Science and Engineering Fair (ASEF), Auburn, Alabama, USA (April 5)

2025** Daniel Pacheco, Regeneron International Science and Engineering Fair (ISEF), Columbus, Ohio (May 10-12)

2025 Andrei Evdokimov, South East Theoretical Chemistry Association Meeting, Memphis, Tennessee, USA (May 8 – 10)

2025 Alexandros Androutsopoulos, South East Theoretical Chemistry Association Meeting, Memphis, Tennessee, USA (May 8 – 10)

2025 Taylor Gregory, South East Theoretical Chemistry Association Meeting, Memphis, Tennessee, USA (May 8 – 10)

2025 Joseph Olaniyan, South East Theoretical Chemistry Association Meeting, Memphis, Tennessee, USA (May 8 – 10)

2025 Andrei Evdokimov, American Chemical Society Fall meeting, Washington, D.C., USA (August 17 – 21)

2025 Alexandros Androutsopoulos, American Chemical Society Fall meeting, Washington, D.C., USA (August 17 – 21)

2025 Ernest C. Agwamba, National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCChE) meeting, Atlanta, GA, USA (September 22 – 25)

2026 Alexandros Androutsopoulos, American Chemical Society Spring meeting, Atlanta, GA, USA (March 22 – 26)

2026 Joseph Olaniyan, American Chemical Society Spring meeting, Atlanta, GA, USA (March 22 – 26)

2026 Taylor Gregory, American Chemical Society Spring meeting, Atlanta, GA, USA (March 22 – 26)

2026* Sydney Risch, American Chemical Society Spring meeting, Atlanta, GA, USA (March 22 – 26)

2026* Samuel Lenz, American Chemical Society Spring meeting, Atlanta, GA, USA (March 22 – 26)

2026 Andrei Evdokimov, South East Theoretical Chemistry Association Meeting, Atlanta, Georgia, USA (May 28 – 30)

2026 Alexandros Androutsopoulos, South East Theoretical Chemistry Association Meeting, Atlanta, Georgia, USA (May 28 – 30)

2026 Taylor Gregory, South East Theoretical Chemistry Association Meeting, Atlanta, Georgia, USA (May 28 – 30)

Oral Presentations of graduate students

2019 Isuru Ariyarathna, 59th Sanibel Symposium, St. Simons Island, Georgia, USA (February 17 – 22)

2019 Shahriar Khan, 59th Sanibel Symposium, St. Simons Island, Georgia, USA (February 17 – 22)

2019 Isuru Ariyarathna, This is Research (student symposium), Auburn, Alabama, USA

2019 Isuru Ariyarathna, 46th National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCChE) meeting, St. Luis, Missouri, USA

2020 Isuru Ariyarathna, 47th National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCChE) virtual meeting

2021 Shahriar Khan, American Chemical Society Spring 2021 virtual meeting (April 5 – 30)

2021 Isuru Ariyarathna, This is Research (student symposium), Auburn, Alabama, USA

2021 Shahriar Khan, SouthEast Regional Meeting of the American Chemical Society (SERMACS), Birmingham, Alabama, USA (November 10-13)

2021 Emily Claveau, SouthEast Regional Meeting of the American Chemical Society (SERMACS), Birmingham, Alabama, USA (November 10-13)

2022 Benjamin Jackson, American Chemical Society Spring 2022 National Meeting, San Diego, California, USA (March 20 – 24)

2022 Emily Claveau, American Chemical Society Fall 2022 National Meeting, Chicago, Illinois, USA (August 21 – 25)

2022 Benjamin Jackson, Swiss Federal Institute of Technology / Eidgenössische Technische Hochschule (ETH) Zürich, Switzerland (October 24)

2022 Benjamin Jackson, Southeastern Universities Graduate Research Symposium, virtual meeting (March 28 – April 1).

2024 Eslam Abdelazim, ACS Local Section Research Symposium, Troy, Alabama, USA (February 23)

2025 Andrei Evdokimov, American Chemical Society Fall meeting, Washington, D.C., USA (August 17 – 21)

Publications in Peer-reviewed Scientific Journals

1. A. Papakondylis, **E. Miliordos** and A. Mavridis, "Carbonyl boron and related systems: An *ab initio* study of B-X and YBBY ($^1\Sigma_g^+$), where X = He, Ne, Ar, Kr, CO, CS, N_2 and Y = Ar, Kr, CO, CS, N_2", *Journal Physical Chemistry A* 108, 4335 (2004), DOI: 10.1021/jp031308q.

2. **E. Miliordos** and A. Mavridis, "The electronic structure of vanadium oxide. Neutral and charged species, $VO^{0,\pm}$", *Journal of Physical Chemistry A* 111, 1953 (2007), DOI: 10.1021/jp067451b.
3. **E. Miliordos**, A. Papakondylis, A. A. Tsekouras and A. Mavridis, "All-electron first principles calculations of the ground and some low-lying excited states of BaI", *Journal Physical Chemistry A* 111, 10002 (2007), DOI: 10.1021/jp0745788.
4. **E. Miliordos** and A. Mavridis, "*Ab initio* investigation of the electronic structure and bonding of BH, BH^-, and HBBH molecules", *Journal of Chemical Physics* 128, 144308 (2008), DOI: 10.1063/1.2902284.
5. **E. Miliordos** and A. Mavridis, "Theoretical study of the early 3d-transition metal diatomic oxides and their ions: $ScO^{0,\pm}$, $TiO^{0,\pm}$, $CrO^{0,\pm}$, $MnO^{0,\pm}$", *Journal of Physical Chemistry A* 114, 8536 (2010), DOI: 10.1021/jp910218u, *Invited Article, Klaus Ruedenberg Festschrift*.
6. **E. Miliordos** and A. Mavridis, "An accurate first principles study of the geometric and electronic structure of B_2, B_2^-, B_3, B_3^-, and B_3H. Ground and excited states", *Journal of Chemical Physics* 132, 164307 (2010), DOI: 10.1063/1.3389133.
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92. B. A. Jackson, S. N. Khan, and **E. Miliordos**, "A fresh perspective on metal ammonia molecular complexes and expanded metals: opportunities in catalysis and quantum information", Chemical Communications, 59, 10572 (2023), DOI: 10.1039/D2CP05480A. *Invited Feature Article, Front Journal Cover, Chemical Communications HOT Article 2023*
93. J. Liu, S. Gao, **E. Miliordos**, and M. Chen, "Asymmetric Syntheses of (Z)- or (E)-β,γ-Unsaturated Ketones via Silane-Controlled Enantiodivergent Catalysis", Journal of American Chemical Society, 145, 19542 (2023), DOI: 10.1021/jacs.3c02595.
94. E. Claveau, E. Heller, J. Richardson, and **E. Miliordos**, "Methane Against Methanol: The Tortoise and the Hare of the Oxidation Race", Journal of Physical Chemistry Letters, 14, 8749 (2023), DOI: 10.1021/acs.jpclett.3c02274.
95. **E. Miliordos**, J. L. Moore, S. V. Obisesan, J. Oppelt, I. Ivanović-Burmazović and C. R. Goldsmith, "Computational Analysis of the Superoxide Dismutase Mimicry Exhibited by a Zinc(II) Complex with a Redox-Active Organic Ligand", Journal of Physical Chemistry A, 128, 1491 (2024), DOI: 10.1021/acs.jpca.3c07403.
96. M. V. White, E. E. Claveau, **E. Miliordos**, and K. D. Vogiatzis, "Electronic Structure and Ligand Effects on the Activation and Cleavage of N_2 on a Molybdenum Center", Journal of Physical Chemistry A, 128, 2038 (2024), DOI: 10.1021/acs.jpca.3c07801. *Invited Article. Roland Lindh Festschrift.*
97. A. Androutsopoulos, S. Sader, and **E. Miliordos**, "Potential of Molecular Catalysts with Electron-Rich Transition Metal Centers for Addressing Long-Standing Chemistry Enigmas", Journal of Physical Chemistry A, 22, 4401 (2024), DOI: 10.1021/acs.jpca.4c01800. *Invited Feature Article.*
98. S. N. Khan, B. Quebedeaux, and **E. Miliordos**, "Selective conversion of methane to methanol facilitated by molecular metal-methoxy complexes via a self-correcting chemical cycle", Physical Chemistry Chemical Physics, 26, 23136 (2024), DOI: 10.1039/D4CP02189D. *Invited Article, PCCP Emerging Investigator.*
99. B. A. Jackson, **E. Miliordos**, and M.-S. Lee, "Theoretical prediction of materials with diffuse electrons with possible applications in redox catalysis and quantum computing", Materials Today Sustainability, 29, 101052 (2024), DOI: 10.1016/j.mtsust.2024.101052. *Invited Article: Special Issue: Materials Design for Sustainable Applications: Insights from Theoretical Simulations.*
100. E. E. Claveau and **E. Miliordos**, "Electronic structure of metal oxide dications with ammonia ligands and their reactivity towards the selective conversion of methane to methanol", Frontiers in Chemistry, 12, 1508515 (2024), DOI: 10.3389/fchem.2024.1508515. *Invited Article: Special Issue: Experimental and Theoretical Studies for Inert C-H Activation.*

101. A. Garayev, E. E. Drake, **E. Miliordos**, R. R. Karimov, "Dearomative Alkylation of Heteroarenium Salts via Blue Light Enabled Homolytic C−C Bond Cleavage", Organic Letters, 27, 1644 (2025), DOI: 10.1021/acs.orglett.4c04831.
102. A. Evdokimov and **E. Miliordos**, "To Transfer or Not to Transfer an Electron: Anionic Metal Centers Reveal Dual Functionality for Polymerization Reactions", Molecules, 30, 1570 (2025), DOI: 10.3390/molecules30071570. *Invited Article: Special Issue: Quantum Chemical Calculations of Molecular Reaction Processes.*
103. M. A. Mohajer, P. Basuri, A. Evdokimov, G. David, D. Zindel, **E. Miliordos**, R. Signorell, "Spontaneous formation of urea from carbon dioxide and ammonia in aqueous droplets", *Science*, 388, 1426 (2025), DOI: 10.1126/science.adv2362.
104. D. P. Vasconcelos, **E. Miliordos**, "On the Selective Conversion of Methane to Methanol Facilitated by Coordinatively Unsaturated Transition Metal Complexes", *Chemistry* 7, 155 (2025), DOI: 10.3390/chemistry7050155. *Invited Article. Journal Cover*
105. A. Evdokimov, V. Nesterova, M. A. Kuroda, K. Klyukin, E. Miliordos, "Electrides with Tunable Electron Delocalization for Applications in Quantum Computing and Catalysis", *ACS Materials Letters* 7, 3604 (2025), DOI: 10.1021/acsmaterialslett.5c00756. *Journal Cover*
106. T. Chiba, J. A. Olaniyan, S. Wang, Y. Han, **E. Miliordos**, K. H. Bowen, "Activation of Methane by Group 11 (Cu, Ag, Au) and Group 9 (Co, Ir) Transition Metal Atomic Anions", *Journal of Physical Chemistry A* 129, 9676 (2025), DOI: 10.1021/acs.jpca.5c04702. *Invited Article. Special Issue: Michael A. Duncan Festschrift*
107. A. Androutsopoulos, **E. Miliordos**, "Reaction of Metal Anionic Centers with Carbon Dioxide: The Case of V^- + CO_2", *Journal of Physical Chemistry A* 129, 10151 (2025), DOI: 10.1021/acs.jpca.5c05663. *Invited Article. Special Issue: Michael A. Duncan Festschrift*
108. A. Androutsopoulos, I. R. Ariyarathna, M. C. Zammit, **E. Miliordos**, A. J. Neukirch, J. A. Leiding, "Low-lying states and total internal partition sums of CH", *Journal of Quantitative Spectroscopy and Radiative Transfer* 352, 109800 (2026), DOI: 10.1016/j.jqsrt.2025.109800
109. B. A. Tufekci, T. Gregory, S. Wang, K. Foreman, T. Chiba, **E. Miliordos**, K. H. Bowen, "Equatorial Ligation Controls 5f Electron Binding in Penta- and Hexavalent Uranyl Acetate Complexes", *Journal of Physical Chemistry A* 9, 1829 (2026), DOI: 10.1021/acs.jpca.6c00067
110. T. Gregory, **E. Miliordos**, "Electronic structure, ligand effects, and chemical reactivity of the ground and low-lying excited electronic states of NpO^{3+}", *Molecules* 31, 1258 (2026), DOI: 10.3390/molecules31081258. *Invited Article: Special Issue: Ab initio Multireference Quantum Chemical Investigations of Molecules: Chemical Bonding, Spectroscopy, and Beyond*
111. T. Chiba, B. R. Bilik, K. Foreman, S. Wang, Y. Han, E. F. M. Abdelazim, S. Sader, **E. Miliordos**, K. H. Bowen, "Partial oxidation of methane to methanol is made possible with metal monoxide anions", *Journal of Chemical Physics* 164, 244303 (2026), DOI: 10.1063/5.0332490
112. J. Olaniyan, D. Pacheco, **E. Miliordos**, "Organometallic Complexes with Electron Rich Metal Centers Promise Efficient and Selective Conversion of Methane to Methanol: Proof of Principle Computational Study", *Frontiers in Catalysis* 6, 1881586 (2026), DOI: XXX

Proposals Funded by Federal Agencies and Auburn University

1. Auburn University New Faculty Start-up Funds
   Award period: June 2016 – indefinite
   Award amount: $400,000
2. National Science Foundation (NSF): “Computational design of Solvated-electron-based Materials for Applications in Redox Chemistry and Quantum Information”
   Principal Investigator: Evangelos Miliordos
   Co-PIs: Marcelo Kuroda, Konstantin Klyukin (Auburn University)
   Award period: September 2025 – August 2028
   Award amount: $672,903
3. National Science Foundation (NSF): “REU: Research Experience in Multiscale Modeling of Matter Embracing Disciplines in Engineering and Sciences”
   Principal Investigator: Marcelo Kuroda
   Co-PI: Konstantin Klyukin (Auburn University)
   Senior-Investigators: Evangelos Miliordos, Eric Burkholder (Auburn University)
   Award period: April 2026 – March 2029
   Award amount: $464,905
4. National Science Foundation (NSF CAREER): “State-of-the-art quantum calculations on a novel class of super-atoms: Discovering exotic chemical bonding schemes and proposing new two- and three-dimensional materials”
   Principal Investigator: Evangelos Miliordos
   Award period: September 2020 – August 2025
   Award amount: $558,374
5. Supplement for International Travel for the NSF CAREER award to support my sabbatical leave (Fall 2022) and visit of one graduate student to ETH-Zürich
   Principal Investigator: Evangelos Miliordos
   Award period: August 2022 – August 2025
   Award amount: $11,340
6. Intramural Grants Program (IGP) – Auburn University: “Multi-scale Modeling of Plasma-Enhanced Semiconducting Nanostructure Synthesis”
   Principal Investigator: Andrew Adamczyk (Department of Chemical Engineering, Auburn U.)
   Award period: August 2020 – July 2022
   Award amount: $50,000
7. Department of Energy: “Tailoring Redox Active Ligands for Probing the Reactivity of Actinides”
   Principal Investigator: Evangelos Miliordos (EPSCoR, inherited from Prof. Anne Gorden)
   Award period: August 2020 – August 2021
   Award amount: $143,010

8. National Energy Research Scientific Computing Center (NERSC): “Ground and excited electronic states of solvated electron precursors”

   Principal Investigator: Evangelos Miliordos

   Award period: August 2018 – August 2020

   Awarded time: 1,350,000 hours

9. National Energy Research Scientific Computing Center (NERSC): “Tailoring Redox Active Ligands for Probing the Reactivity of Actinides”

   Principal Investigator: Evangelos Miliordos

   Award period: October 2020 – January 2022

   Awarded time: 1,550,000 hours

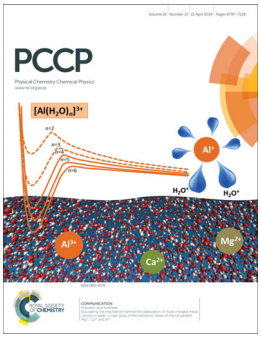
10. College of Sciences and Mathematics center: “CM^4: Center for Multiscale Modeling of Materials and Molecules”

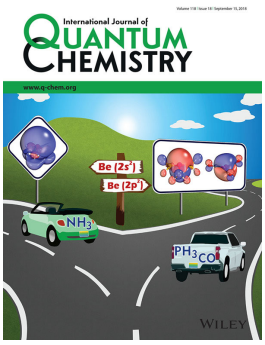
    Principal Investigators: Evangelos Miliordos & Marcelo Kuroda (Department of Physics, Auburn University)

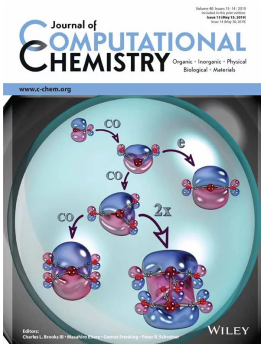
    Award period: January 2024 – December 2025

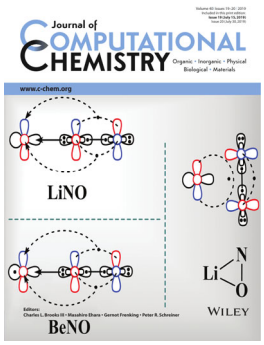
    Award amount: $32,000

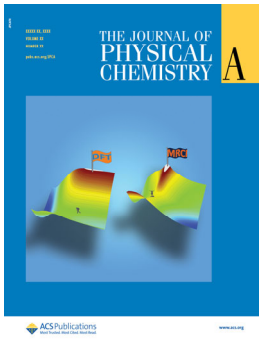
Journal Covers

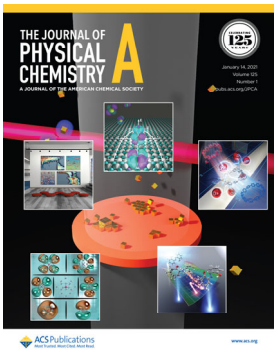


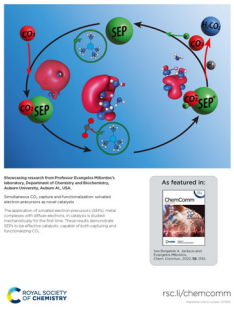


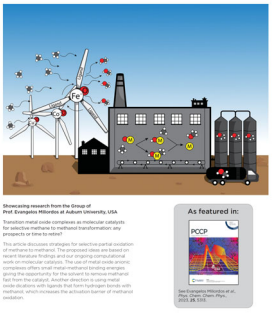


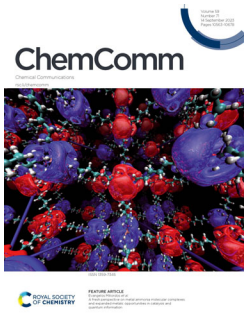


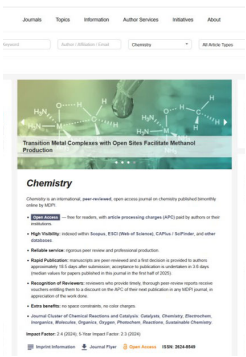












Other Publications

1. **E. Miliordos**, "*Ab initio* calculations on the ethane molecule and its cation", *Diploma Thesis*, Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece (2003).
2. **E. Miliordos**, "Theoretical investigation of the vanadium oxides, $VO^{0,\pm}$", *Master Thesis*, Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece (2006).
3. **E. Miliordos**, "Electronic structure of the $MO^{0,\pm}$ oxides, M = Sc, Ti, Cr, Mn, through *ab initio* calculations", *Ph. D. Thesis*, Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece (2010).