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

Professional Employment

August 2020 – today	***Director of the Physical Chemistry Division*** Department of Chemistry and Biochemistry Auburn University Auburn, Alabama, USA
August 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 – July 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	***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 postgraduate 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)

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 – present AICHE member ID: 009904802549
Association of Greek Chemists, 2003 – 2008

Teaching Experience

Auburn University: *CHEM 1030* General Chemistry I (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 7330 Chemical kinetics (graduate 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)

Students and Post-doctoral Researchers Mentored

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-present)
Andrei Evdokimov (2023-present)
Alexandros Androutsopoulos (2023-present)

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-present)

Post-doctoral Researchers:

Nuno Almeida (2017-2019)

Achievements of Graduate 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)

Reviewing Activities

Journals: The Journal of Chemical Physics, Chemical Physics, Journal of Quantitative Spectroscopy and Ratiative Transfer, Chemical Physics Letters, The Journal of Physical Chemistry, 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, Journal of Chemical Education

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

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)

Citation Index

Google Scholar: Total of 1886 citations (as of August 15th, 2023) Hirsch index: 24

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)

Professional Service

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

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)

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 Contributed Talk, 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 Heavy Element Chemistry Principal Investigators' Meeting, Washington DC, USA (April 23-25)

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

Poster Presentations of graduate 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 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)

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).

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.
7. **E. Miliordos**, "Hückel versus Möbius aromaticity: The particle in a cylinder versus a Möbius strip", *Physical Review A* 82, 062118 (2010), DOI: 10.1103/PhysRevA.82.062118. Highlighted in *Science News* issue of January 29, 2011 (page 16), https://www.sciencenews.org/article/twisted-rules-chemistry-explained.
8. **E. Miliordos** and K. L. C. Hunt, "First principles calculations of the electronic and geometrical structures of neutral [Sc,O,H] molecules and the monocations, $ScOH^{0,+}$ and $HScO^{0,+}$", *Journal of Physical Chemistry A* 115, 4436 (2011), DOI: 10.1021/jp110378d.
9. **E. Miliordos**, "The particle in a Möbius wire and half-integer orbital angular momentum", *Physical Review A* 83, 062107 (2011), DOI: 10.1103/PhysRevA.83.062107.
10. C. N. Sakellaris, **E. Miliordos** and A. Mavridis, "First principles study of the ground and excited states of FeO, FeO^+, and FeO^-", *Journal of Chemical Physics* 134, 234308 (2011), DOI: 10.1063/1.3598529.
11. **E. Miliordos**, J. F. Harrison and K. L. C. Hunt, "*Ab initio* investigation of titanium hydroxide isomers and their cations, $TiOH^{0,+}$ and $HTiO^{0,+}$", *Journal of Chemical Physics* 135, 144111 (2011), DOI: 10.1063/1.3644963.
12. X. Li, A. Mandal, **E. Miliordos** and K. L. C. Hunt, "Interaction-induced dipoles of hydrogen molecules colliding with helium atoms: A new *ab initio* dipole surface for high-temperature applications", *Journal of Chemical Physics* 136, 044320 (2012), DOI: 10.1063/1.3676406.
13. **E. Miliordos**, J. F. Harrison and K. L. C. Hunt, "Ground and excited states of vanadium hydroxide isomers and their cations, $VOH^{0,+}$ and $HVO^{0,+}$", *Journal of Chemical Physics* 138, 114305 (2013), DOI: 10.1063/1.4793744.
14. **E. Miliordos** and J. F. Harrison, "Hirshfeld density partitioning technique: a first application on transition metal compounds, TiO, VO, ScOH", *Journal of Chemical Physics* 138, 184305 (2013), DOI: 10.1063/1.4803478.
15. **E. Miliordos**, K. Ruedenberg and S. S. Xantheas, "Unusual inorganic biradicals: A Theoretical Analysis", Communication to the Editor, *Angewandte Chemie International Edition* 52, 5736 (2013), DOI: 10.1002/anie.201300654.
16. **E. Miliordos** and S. S. Xantheas, "Efficient procedure for the numerical calculation of harmonic vibrational frequencies based on internal coordinates", *Journal of Physical Chemistry A* 117, 7019 (2013), DOI: 10.1021/jp3127576, *Invited Article, Joel M. Bowman Festschrift*.
17. **E. Miliordos**, E. Aprà and S. S. Xantheas, "Optimal geometries and harmonic vibrational frequencies of the global minima of water clusters $(H_2O)_n$, n=2-6, and several hexamer local minima at the CCSD(T) level of theory" *Journal of Chemical Physics* 139, 114302 (2013), DOI: 10.1063/1.4820448.
18. **E. Miliordos** and S. S. Xantheas, "Elucidating the mechanism behind the stabilization of multi-charged metal cations in water: A case study of the electronic states of microhydrated Mg^{2+}, Ca^{2+} and Al^{3+}", Hot article for the week Oct 22, 2013 (http://blogs.rsc.org/cp/2013/10/22/this-weeks-hot-articles-11/), Highlighted in NERSC's web page, June 2014, http://www.nersc.gov/news-

publications/news/science-news/2014/thirsty-metals-key-to-longer-battery-lifetimes/. Highlighted in DOE's Pulse (Science and Technology Highlights from the DOE National Laboratories, #417, 7 July 2014 http://web.ornl.gov/info/news/pulse/no417/story1.shtml. Reported in Science Springs, July 7 2014 http://sciencesprings.wordpress.com/2014/07/07/from-doe-pulse-satisfying-metals-thirst-vital-for-high-capacity-batteries/, Communication to the Editor, *Physical Chemistry Chemical Physics* 16, 6886 (2014), DOI: 10.1039/c3cp53636j. *Journal cover*

19. **E. Miliordos** and S. S. Xantheas, "Unimolecular and hydrolysis channels for the detachment of water from microsolvated alkaline earth dication (Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}) clusters", *Theoretical Chemistry Accounts* 133, 1450 (2014), DOI: 10.1007/s00214-014-1450-4, *Invited Article, Thom H. Dunning Jr. Festschrift*.
20. **E. Miliordos** and S. S. Xantheas, "On the bonding nature of ozone (O_3) and its sulfur-substituted analogues, SO_2, OS_2, and S_3: Correlation between their biradical character and molecular properties", *Journal of the American Chemical Society* 136, 2808 (2014), DOI: 10.1021/ja410726u.
21. **E. Miliordos**, E. Aprà and S. S. Xantheas, "Benchmark Theoretical Study of the π−π Binding Energy in the Benzene Dimer" *Journal of Physical Chemistry A* 118, 7568 (2014), DOI: 10.1021/jp5024235.
22. N. Sahu, S. R. Gadre, A. Rakshit, P. Bandyopadhyay, **E. Miliordos** and S. S. Xantheas, "Low energy isomers of $(H_2O)_{25}$ from a hierarchical method based on Monte Carlo temperature basin paving and molecular tailoring approaches benchmarked by MP2 calculations" *Journal of Chemical Physics* 141, 164304 (2014), DOI: 10.1063/1.4897535.
23. J. C. Werhahn, **E. Miliordos** and S. S. Xantheas, "A new variation of the Buckingham exponential-6 potential with a tunable, singularity-free short-range repulsion and an adjustable long-range attraction", *Chemical Physics Letters* 619, 153 (2015), DOI: 10.1016/j.cplett.2014.11.051.
24. T. Karman, **E. Miliordos**, K. L. C. Hunt, G. C. Groenenboom and Ad van der Avoird, "Quantum mechanical calculation of the collision-induced absorption spectra of N_2–N_2 with anisotropic interactions", *Journal of Chemical Physics* 142, 084306 (2015), DOI: 10.1063/1.4907917.
25. **E. Miliordos** and S. S. Xantheas, "On the validity of the basis set superposition error and complete basis set limit extrapolations for the binding energy of the formic acid dimer", *Journal of Chemical Physics* 142, 094311 (2015), DOI: 10.1063/1.4913766.
26. **E. Miliordos** and S. S. Xantheas, "Ground and excited states of the $[Fe(H_2O)_6]^{2+}$ and $[Fe(H_2O)_6]^{3+}$ clusters: Insight into the electronic structure of the $[Fe(H_2O)_6]^{2+}$–$[Fe(H_2O)_6]^{3+}$", *Journal of Chemical Theory and Computation* 11, 1549 (2015), DOI: 10.1021/ct501143c.
27. **E. Miliordos** and S. S. Xantheas, "An accurate and efficient computational protocol for obtaining the complete basis set limits of the binding energies of water clusters at the MP2 and CCSD(T) levels of theory: Application to $(H_2O)_m$, m = 2-6, 8, 11, 16, and 17", *Journal of Chemical Physics* 142, 234303 (2015), DOI: 10.1063/1.4922262.
28. **E. Miliordos** and S. S. Xantheas, "The origin of the reactivity of the Criegee intermediate: implications for atmospheric particle growth", *Angewandte Chemie International Edition* 55, 1015 (2016), DOI: 10.1002/anie.201509685.
29. C. T. Wolke, J. A. Fournier, **E. Miliordos**, S. M. Kathmann, S. S. Xantheas, and M. A. Johnson, "Isotopomer-selective spectra of a single intact H_2O molecule in the $Cs^+(D_2O)_5H_2O$ isotpologue:

Going beyond pattern recognition to harvest the structural information encoded in vibrational spectra", *Journal of Chemical Physics* 144, 074305 (2016), DOI: 10.1063/1.4941285.

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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 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
3. 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
4. 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
5. 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
6. 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

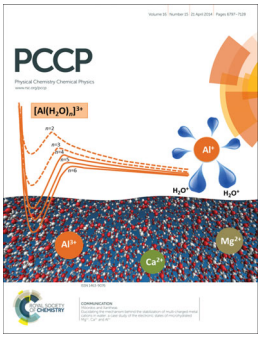
7. National Energy Research Scientific Computing Center (NERSC): “Tailoring Redox Active Ligands for Probing the Reactivity of Actinides”

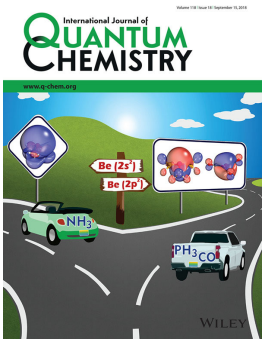
   Principal Investigator: Evangelos Miliordos

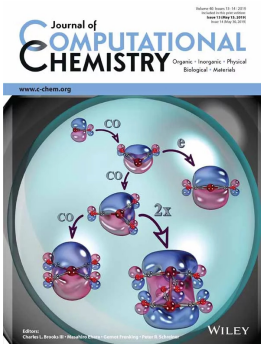
   Award period: October 2020 – January 2022

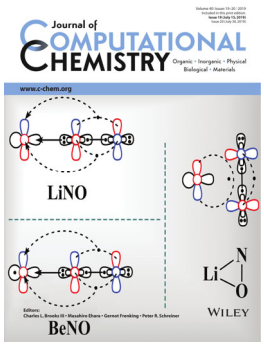
   Awarded time: 1,550,000 hours

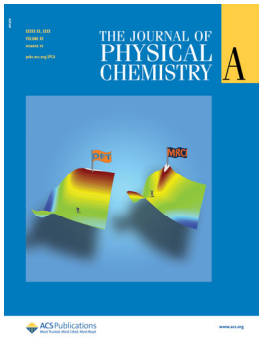
Journal Covers

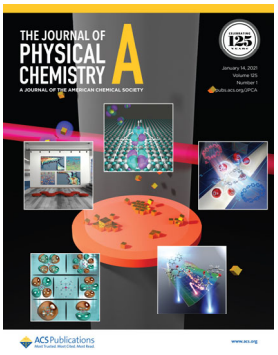


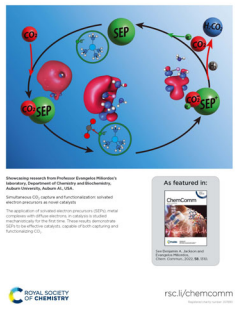


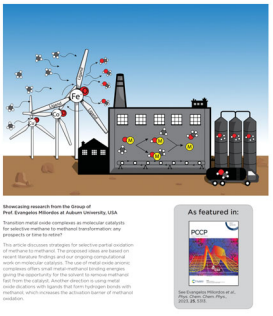


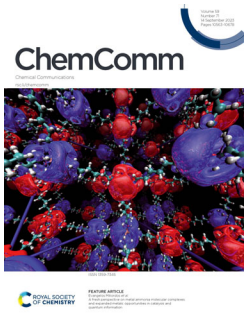












Other Publications

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).