CURRICULUM VITAE

NAME: Laimutis Bytautas

CURRENT POSITION: Adjunct Faculty/Professor.

ADDRESS AND CONTACT INFORMATION:

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EDUCATION:

1991-1996 Ph. D. in Physical Chemistry. Vanderbilt University, Nashville, TN, USA.
Dissertation title: "Theoretical Studies of Chemical Reactions".

1983-1990 M.Sc. in Physics. Vilnius University, Vilnius, Lithuania.
Thesis title: "Investigation of discreate gluonic-field spectrum using SU(2) model Hamiltonian".

PROFESSIONAL EXPERIENCE:

2013 - present Adjunct Faculty/Professor.
Chemistry Department, Houston Community College, Houston, TX.

2012 - present Adjunct Faculty/Professor.
Physics Department, Texas Southern University, Houston, TX.

2010-present Research Associate (not on payroll).
Iowa State University, Ames Laboratory USDOE, Ames, IA, USA.

2012-fall Adjunct Faculty.
Chemistry Department, Lone Star College, CyFair, Cypress, TX.

2012-fall Research Associate (part-time).
Baylor College of Medicine, Pharmacology Department, Houston, TX.

2011 – 2012 *Senior Research Associate*.
Department of Chemistry, Rice University, Houston, TX, USA.

2010 – 2011 *Research Scientist*.
Department of Chemistry, Rice University, Houston, TX, USA.

2003 – 2010 *Assistant Scientist*.
Iowa State University, Ames Laboratory USDOE, Ames, IA, USA.

1999 – 2003 *Postdoctoral Research Associate*.
Iowa State University, Ames Laboratory USDOE, Ames, IA, USA.

1996 – 1999 *Postdoctoral Research Associate*.
Department of Marine Sciences, Texas A&M University at Galveston, TX, USA.

1990 – 1991 *Research Associate*,
Institute of Theoretical Physics and Astronomy, Vilnius, Lithuania.

TEACHING AND SUPERVISION EXPERIENCE:

2013 – present *Adjunct Faculty/Professor*. Department of Biology and Physical Science. Houston Community College (Central). 1300B Holman St. Houston, TX.

2012 – present *Adjunct Faculty/Professor*. Department of Physics, Texas Southern University, 3100 Cleburne Av., Houston, TX.

2012 – fall *Adjunct Faculty*. Chemistry Department, Lone Star College, CyFair, 9191 Barker Cypress Road, Cypress, TX.

2003 – 2012 Mentoring of postdoctoral scholars and graduate students.

1991 – 1996 *Teaching Assistant*. General Chemistry and Physical Chemistry Labs, Vanderbilt University, Nashville, TN.

COMPETETIVE HONORS AND AWARDS:

2012 Approval of the Symposium proposal at the Southwest Regional American Chemical Society meeting in Baton Rouge, LA, USA. Nov. 4-7, 2012. Title: "*Conjugated-Carbon Nanostructures: Molecular Topology, Tunable Properties and Applications*". The budget: $2000.

LEADERSHIP:

- *Lead Guest Editor*: Special Issue in *Advances in Physical Chemistry*. "*Accurate Potential Energy Surfaces and Beyond: Chemical Reactivity, Binding, Long Range Interactions and Spectroscopy*" (2011-2012).
- *Organizer of the Symposium*: "*Conjugated-Carbon Nanostructures: Molecular Topology, Tunable Properties and Applications*"[with D. J. Klein]. Southwest Regional ACS Meeting in Baton Rouge, LA, USA. Nov. 4-7, 2012.
- *Member of the Editorial Board*: *ISRN Physical Chemistry*. (2011-present).
- *Member of the Editorial Board*: *The SciTech, Journal of Science and Technology*, (2012-present).

PROFESSIONAL SERVICE:

- *Reviewer* for the scientific research journals:
  Journal of Physical Chemistry.
  Chemical Physics Letters.
  Journal of Chemical Physics.
  Journal of Chemical Theory and Computation.
  Communications in Mathematical and in Computer Chemistry (MATCH).
  Journal of Computational Chemistry.
  International Journal of Molecular Sciences.
  Nature (Scientific Reports).

PROFESSIONAL MEMBERSHIPS:

- Member of the American Chemical Society (ACS) since 2001.

RESEARCH INTERESTS AND HIGHLIGHTS:

- Developer of *ab initio* Quantum Chemistry methodology (theory and computer codes).
- Inventor of a new *ab initio* method: CEEIS-FCI (with K. Ruedenberg). CEEIS-FCI code is currently available in GAMESS *ab initio* quantum chemistry program package.
- Ab initio rotational-vibrational spectroscopy: First accurate ab initio potential energy curves (using CEEIS-FCI method) yielding near-spectroscopic accuracy for the rotational-vibrational spectrum of the molecules: F_2, O_2 and B_2.
- Physical and chemical properties of nanomaterials.
- Toxic compounds in the environment and their reactivity.
- Structure-property, structure-activity relationships with biochemical and biomedical implications.
- Kinetic isotope effects and transition metal chemistry.

IMPACT OF RESEARCH PUBLICATIONS:

- **Google Scholar:** Total number of citations: **788 (February 14, 2013).**

LIST OF PUBLICATIONS (40):

- L. Bytautas, J. M. Bowman, X. Huang, A.J.C. Varandas, "Editorial: Accurate Potential Energy Surfaces and Beyond: Chemical Reactivity, Binding, Long-Range Interactions, and Spectroscopy", Advances of Physical Chemistry vol. **2012**, Article ID 679869 (2012).
- L. Bytautas, N. Matsunaga, G. E. Scuseria, K. Ruedenberg, "Accurate potential energy curve for B_2. *Ab initio* elucidation of the experimentally elusive ground state rotation-vibration spectrum", Journal of Physical Chemistry A, **116**, 1717 (2012).
- L. Bytautas, T. M. Henderson, C. A. Jiménez-Hoyos, J. Ellis and G. E. Scuseria, "Seniority and orbital symmetry as tools for establishing a full configuration interaction hierarchy", Journal of Chemical Physics **135**, 044119 (2011).
- L. Bytautas, K. Ruedenberg, "The range of electron correlation between localized molecular orbitals. A full configuration interaction analysis for the NCCN molecule" J. Phys. Chem. A **114**, 8601 (2010). [invited article for the special issue in honor of Klaus Ruedenberg].
- L. Bytautas, K. Ruedenberg, "Accurate ab initio Potential Energy Curve of O_2. I. Nonrelativistic Full Configuration Interaction Valence Correlation using the CEEIS method" J. Chem. Phys. **132**, 074109 (2010).
- L. Bytautas, N. Matsunaga, K. Ruedenberg, "Accurate ab initio Potential Energy Curve of O_2. II. Core-valence Correlations, Relativistic Contributions and the Vibrational-Rotation Spectrum" J. Chem. Phys. **132**, 074307 (2010).

- L. Bytautas, K. Ruedenberg, "Ab initio potential energy curve of F_2. IV. Transition from the covalent to the van der Waals region: Competition between multipolar and correlation forces" J. Chem. Phys. **130**, 204101 (2009).
- L. Bytautas, K. Ruedenberg, "A priori identification of configurational deadwood" Chemical Physics **356**, 64 (2009).
- L. Bytautas, K. Ruedenberg, "Correlation Energy and Dispersion Interaction in the ab initio Potential Energy Curve of the Neon Dimer" J. Chem. Phys. **128**, 214308 (2008).
- L. Bytautas, T. Nagata, M. S. Gordon, K. Ruedenberg, "Accurate ab initio Potential Energy Curve of F_2. I. Nonrelativistic Full Valence Configuration Interaction Energies using the Correlation Energy Extrapolation by Intrinsic Scaling" J. Chem. Phys. **127**, 164317 (2007).
- L. Bytautas, N. Matsunaga, T. Nagata, M. S. Gordon, K. Ruedenberg, "Accurate ab initio Potential Energy Curve of F_2. II. Core-valence Correlations, relativistic contributions, and long-range interactions" J. Chem. Phys. **127**, 204301 (2007).
- L. Bytautas, N. Matsunaga, T. Nagata, M. S. Gordon, K. Ruedenberg, "Accurate ab initio Potential Energy Curve of F_2. III. The Vibration Rotation Spectrum" J. Chem. Phys. **127**, 204313 (2007).
- L. Bytautas, K. Ruedenberg, "Economical Description of Electron Correlation" in Electron Correlation Methodology, ACS Symposium Series vol. **958**, p. 103-123, Eds. A. K. Wilson and K. A. Peterson, American Chemical Society, Washington DC (2007).[**Book Chapter**].
- L. Bytautas, K. Ruedenberg, "Correlation Energy Extrapolation by Intrinsic Scaling. V. Electronic Energy, Atomization Energy, and Enthalpy of Formation of Water" J. Chem. Phys. **124**, 174304 (2006).
- M. S. Gordon, K. Ruedenberg, M. W. Schmidt, L. Bytautas, T. J. Dudley, T. Nagata, R. Olson, S. Varganov, "Scalable Correlated Electronic Structure Theory" Journal of Physics: Conference Series **46**, 229-233 (2006).
- L. Bytautas, K. Ruedenberg "Correlation Energy Extrapolation by Intrinsic Scaling. IV. Accurate Binding Energies of the Homonuclear Diatomic Molecules Carbon, Nitrogen, Oxygen and Fluorine", J. Chem. Phys. **122**, 154110 (2005).
- L. L. Griffin, Jian Wu, D. J. Klein, T. G. Schmalz, L. Bytautas, "Scaling behaviour of Ground-State Energy Cluster Expansion for Linear Polyenes" International Journal of Quantum Chemistry **102**, 387 (2005).
- L. Bytautas, K. Ruedenberg "Correlation Energy Extrapolation by Intrinsic Scaling. I. Method and Application to the Neon atom", J. Chem. Phys. **121**, 10905 (2004).
- L. Bytautas, K. Ruedenberg "Correlation Energy Extrapolation by Intrinsic Scaling. II. The water and the nitrogen molecule", J. Chem. Phys. **121**, 10919 (2004).
- L. Bytautas, K. Ruedenberg "Correlation Energy Extrapolation by Intrinsic Scaling. III. Compact Wave Functions", J. Chem. Phys. **121**, 10852 (2004).
- W. C. Lu, C. Z.Wang, M. W. Schmidt, L. Bytautas, K. M. Ho, K. Ruedenberg,

"Molecule Intrinsic Minimal Basis Sets.I. Exact Resolution of Ab initio Optimized Molecular Orbitals in terms of deformed Atomic Minimal-Basis Orbitals" Journal of Chemical Physics **120**, 2629 (2004).

- W. C. Lu, C. Z.Wang, M. W. Schmidt, L. Bytautas, K. M. Ho, K. Ruedenberg, "Molecule Intrinsic Minimal Basis Sets.II. Bonding Analyses in Si_4H_6 and Si_2 to Si_{10}" Journal of Chemical Physics **120**, 2638 (2004).
- L. Bytautas, J. Ivanic, K. Ruedenberg, "Split-localized orbitals can yield stronger configuration interaction convergence than natural orbitals", Journal of Chemical Physics **119**, 8217 (2003).
- L. Bytautas, K. Ruedenberg, "Electron pairs, localized orbitals and electron correlation", Molecular Physics **100**, 757 (2002).
- O. Ivanciuc, L. Bytautas, D. J. Klein, "Mean-field resonating-valence-bond theory for unpared π-electrons in benzenoid carbon species", Journal of Chemical Physics **116**, 4735 (2002).
- O. Ivanciuc, D. J. Klein, L. Bytautas, "Unpaired π-spin density in defected graphite", Carbon **40**, 2063 (2002).
- L. Bytautas, D. Bonchev, D. J. Klein, "On the Generation of Mean Wiener Numbers of Thorny graphs" Commun. in mathematical and in computer chemistry (MATCH) **44**, 31 (2001).
- L. Bytautas, D. J. Klein, M. Randić and T. Pisanski, "Foldedness in Linear Polymers: A Difference between Graphical and Euclidean Distances", DIMACS Series in Discrete Mathematics and Theoretical Computer Science **51**, 39 (2000). [**Book Chapter**].
- L. Bytautas and D. J. Klein, "Formula Periodic Table for the Isomer Classes of Acyclic Hydrocarbons – Enumerative and Asymptotic Characteristics" Croatica Chemical Acta. **73**, 331 (2000).
- L. Bytautas, D. J. Klein, T. G. Schmalz, "All acyclic hydrocarbons: formula periodic table and property overlap plots via chemical combinatorics", New Journal of Chemistry **24**, 329 (2000).
- D. J. Klein and L. Bytautas, "Directed Reaction Graphs as Posets" Commun. in mathematical and in computer chemistry (MATCH) **42**, 261 (2000).
- L. Bytautas and D. J. Klein, "Mean Wiener Numbers and Other Mean Extensions for Alkane Trees", J. Chemical Information & Computer Science **40**, 471 (2000).
- L. Bytautas and D. J. Klein, "Isomer Combinatorics for Acyclic Conjugated Polyenes: Enumeration and Beyond", Theoretical Chemistry Accounts **101**, 371 (1999).
- D. J. Klein and L. Bytautas, "Graphitic Edges and Unpaired π-electron Spins", Journal of Physical Chemistry A **103**, 5196 (1999).
- L. J. Schaad, L. Bytautas, and K. N. Houk, "Ab initio Test of the Usefulness of the Redlich-Teller Product Rule in Computing Kinetic Isotope Effects", Canadian Journal of Chemistry **77**, 875 (1999).

- D. J. Klein, T. G. Schmalz and L. Bytautas, "Chemical Sub-structural Cluster Expansions for Molecular Properties", SAR and QSAR in Environmental Research **10**, 131 (1999).
- L. Bytautas and D. J. Klein, "Alkane Isomer Combinatorics – Stereostructure Enumeration, Graph-invariant & Molecular Property Distributions", J. Chemical Information & Computer Science **39**, 803 (1999).
- L. Bytautas and D. J. Klein, "Formula Periodic Table for Acyclic Hydrocarbon Isomer Classes: Combinatorially Averaged Graph-Invariants", Physical Chemistry Chemical Physics **1**, 5565 (1999).
- L. Bytautas and D. J. Klein, "Chemical Combinatorics for Alkane-Isomer Enumeration and More", J. Chemical Information & Computer Science **38**, 1063 (1998).
- L. Bytautas and D. J. Klein, "Symmetry Aspects of Nonrigid Molecules and Transition Structures in Chemical Reactions", International J. Quantum Chem. **70**, 205 (1998).

PRESENTATIONS:

- **Symposium talk:** "Symposium on conjugated-carbon nanostructures: Molecular topology, tunable properties and applications*"*
  L. Bytautas and D. J. Klein: Presented on November 4, **2012** at the Southwest Regional American Chemical Society meeting in Baton Rouge, LA, USA. Nov. 4-7, 2012. USA.

- **Invited seminar:** "*Ab initio Method Development and Applications: Theoretical predictions of vibrational spectrum ahead of spectroscopic measurement"*
  L. Bytautas: Presented on April 26, **2012** at the Department of Physics, Texas Southern University, Houston, TX, USA.

- **Invited talk:** "*Theoretical ab initio predictions of vibrational spectrum ahead of spectroscopic measurement"*
  L. Bytautas, N. Matsunaga, K. Ruedenberg, G. E. Scuseria, presented at the 24-th *Symposium on Molecular Structure and Dynamics* in Dallas, TX, USA. March 3-6, **2012**. Invitation by Professor Elfi Kraka (Southern Methodist University, Conference Organizer).

- **Invited seminar:** "*Ab initio Method Development and Applications: Solving Challenging Problems in Today's World*"
  L. Bytautas: Presented on September 27, **2011** at the Department of Oceanography, Texas A&M University at Galveston, Galveston, TX, USA.

- **Talk:** "*New ab initio approaches for accurate description of the bond breaking: How close are we to the "spectroscopic accuracy"?* "
  L. Bytautas, N. Matsunaga, K. Ruedenberg, G. E. Scuseria, M. S. Gordon, T. Nagata, the Ninth Triennial Congress of the WORLD ASSOCIATION OF THEORETICAL AND COMPUTATIONAL CHEMISTS: WATOC 2011, Santiago de Compostela, SPAIN, July 20, **2011**.

- **Poster** at Psi-k-Conference 2010, held in Berlin, GERMANY, September 12-16, **2010**.

L. Bytautas, K. Ruedenberg, N. Matsunaga, M. S. Gordon, T. Nagata, G. E. Scuseria "New ab initio approaches for accurate description of the bond breaking processes"

- **Poster** at 22-nd Annual Workshop on Electronic Structure Methods, held in University of Texas, Austin, TX, USA, June 7-10, **2010**. L. Bytautas, K. Ruedenberg, N. Matsunaga, G. E. Scuseria "New ab initio approaches for accurate description of the bond breaking processes"

- **Poster** at XIII-th International Congress of Quantum Chemistry held in Helsinki, FINLAND, June 22-27, **2009**.
L. Bytautas, K. Ruedenberg "Accurate calculations of the reaction paths for diatomic molecules using CI wavefunctions"

- **Poster** at XII-th International Congress of Quantum Chemistry held in Kyoto, JAPAN, May 21-26, **2006**.
L. Bytautas, N. Masunaga, T. Nagata, M. S. Gordon, K. Ruedenberg
"Beyond chemical accuracy along reaction paths"

- **Talk** at the 230-th American Chemical Society National Meeting held in Washington DC, USA, August 28-September 1, **2005**. Symposium on Computational Exploration of Energy Landscapes: Challenges and Solutions
L. Bytautas, K. Ruedenberg, T. Nagata, M. S. Gordon "Towards Chemical Accuracy for non-equilibrium structures of molecules".

- **Talk** at the 228-th American Chemical Society National Meeting held in Philadelphia, PA, USA, August 22-26, **2004**.
L. Bytautas and K. Ruedenberg, "Correlation Energy Extrapolation by Intrinsic Scaling".

- **Talk** at the 36-th Midwest Theoretical Chemistry Conference at Michigan State University, East Lansing, MI, USA, June 17-19, **2004**.
L. Bytautas, K. Ruedenberg, "Correlation Energy Extrapolation by Intrinsic Scaling".

- **Talk** at the 226-th American Chemical Society National Meeting held in New York, NY, USA, September 7-11, **2003**. *Symposium on Making and Breaking Chemical Bonds in Gas and Condensed Phases: Theory and Applications:*
L. Bytautas and K. Ruedenberg, "Large Full Valence Spaces Without Configurational Deadwood".

- **Talk** at the 35-th Midwest Theoretical Chemistry Conference at Iowa State University, Ames, IA, USA, June 12-14, **2003**. L. Bytautas, K. Ruedenberg, "A priori elimination of all configurational deadwood from large full valence spaces".

- **Invited physical chemistry seminar** at Iowa State University, USA, May 9, **2003**.
L. Bytautas, "Electron Pairs, Localized Orbitals and Electron Correlation".

- **Poster** presented at 11-th American Conference on Theoretical Chemistry (ACTC'02),

July 13-18, Champion, PA, USA, **2002**.
L. Bytautas, J. Ivanic, K. Ruedenberg "A priori elimination of configurational deadwood from large full valence spaces by use of localized orbitals"

- **Talk** at the 223-rd American Chemical Society National Meeting held in Orlando, FL, USA. April 7-11, **2002**. Symposium: Recent Advances in Electron Correlation Methodology:
L. Bytautas, J. Ivanic, K. Ruedenberg, "Compact description of correlation using localized orbitals".

- **Poster** presented in 34th Midwest Theoretical Chemistry Conference, MN, USA, October 5-6, **2001**.
L. Bytautas, K. Ruedenberg "Back-of-the envelope predictions of correlation energies".

- **Poster** presented at 10th American Conference on Theoretical Chemistry (ACTC'99), June 27-July 2, Boulder, Colorado, USA, **1999**. L. Bytautas and D. J. Klein "Formula Periodic Table for Acyclic Hydrocarbon Isomer Classes - Combinatorially Averaged Properties".

- **Talk** presented at 15th Southwest Theoretical Chemistry Conference, Denton, TX, USA, November, **1998**: L. Bytautas and D. J. Klein, "Alkane Combinatorics"

- **Talk** presented at 14th Southwest Theoretical Chemistry Conference, New Orleans, LA, USA, November, **1997**: L. Bytautas and D. J. Klein, "Acyclic Polyene Isomer Enumeration and Beyond"

- **Poster** presented at the 9th International Congress Of Quantum Chemistry (ICQC-IX), Atlanta, GA, USA, June **1997**: L. Bytautas and L. J. Schaad, "General Symmetry Rules for Transition Structures in Chemical Reactions".

- **Poster** presented at 25th Southeastern Theoretical Chemistry Association Conference (SETCA), Tallahassee, FL, USA, May **1996**: L. Bytautas and L. J. Schaad, "Need a Reaction Path Leave Reactant Along One of the Normal Coordinates?"

- **Talk** presented in 47th Southeast-51th Southwest Joint Regional Meeting of American Chemical Society, Memphis, TN, USA, November **1995**: L. Bytautas and L. J. Schaad, " Determination of Transition Structure Symmetry in Degenerate Chemical Reactions"

- **Talk** presented at the 24th (SETCA) Conference, New Orleans, LA, USA, May **1995**: L. Bytautas and L. J. Schaad, "Symmetry Rules for Transition Structures in Chemical Reaction: a case where the Murrell-Laidler theorem is not assumed to hold"

- **Poster** presented at the 23d (SETCA) Conference, Nashville, TN, USA, May **1994**: L. J. Schaad and L. Bytautas, "Usefulness of the Redlich-Teller Product Rule in Reducing the Error in Calculated KIE: the ab initio computational test",

- **Poster** presented at the 22nd (SETCA) Conference, Raleigh, NC, USA, May **1993**: L. Bytautas and L. J. Schaad, "The influence of π-electron delocalization on the tendency of the molecule to maintain CC bonds of equal length in hydrocarbons".