Laimutis Bytautas
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Search for Classes

QUALIFICATION
Vanderbilt University
Doctorate - Chemistry
December 1996

Vilniaus University
Bachelor - Physics
August 1990

POSITIONS HELD
Galveston College
Adjunct Instructor of Chemistry
2013

Houston Community College
Adjunct Instructor of Chemistry
2013

Texas Southern University
Adjunct Instructor of Physics
2012 to 2013

Lone Star College, CyFair
Adjunct Instructor of Chemistry
2012 to 2013

Baylor College of Medicine
Research Associate
October 2012 to November 2012

Rice University
Senior Research Associate/Research Scientist
February 2010 to August 2012

Iowa State University
Assistant Scientist/Postdoctoral Research Associate
1999 to 2010

Texas A&M University at Galveston
Postdoctoral Research Associate
1996 to 1999

PUBLICATIONS

Laimutis Bytautas and Jorge Dukelsky, "Seniority based energy renormalization group (Ω-ERG) approach in quantum chemistry: Initial formulation and application to potential energy surfaces." Computational and Theoretical Chemistry, Volume 1141, 1 October 2018, Pages 74-88 (2018).

D. Bhattacharya, S. Shil, A. Misra, L. Bytautas, D. J. Klein, "Toward Molecular Magnets of Organic Origin via Anion-π Interaction Involving *m*-aminyl diradical: A Theoretical Study " *The Journal of Physical Chemistry A* **120**, 9117-9130 (2016).

L. Bytautas, G. E. Scuseria, K. Ruedenberg
"Seniority number description of potential energy surfaces: symmetric dissociation of water, N2, C2, and Be2". Journal of Chemical Physics 143, 094105 (2015).

D. Bhattacharya, S. Shil, A. Misra, L. Bytautas, D. J. Klein "Photomagnetic and Non Linear Optical Properties in cis-trans Green Fluoroprotein Chromophore Coupled Bis-Imino Nitroxide Diradicals."
International Journal of Quantum Chemistry 115, 1561 (2015).

D. Bhattacharya, S. Shil, A. Misra, L. Bytautas, D. J. Klein "Borazine: spin blocker or not? "
Phys. Chem. Chem. Phys. 17, 14223 (2015).

L. Bytautas, C. A. Jiménez-Hoyos, R. Rodríguez-Guzmán and G. E. Scuseria
"Potential energy curves for Mo2: multi-component symmetry-projected Hartree–Fock and beyond."
Molecular Physics 112, 1938 (2014).

L. Bytautas "Stability of dimethylmercury and related mercury-containing compounds with respect to selected chemical species found in aqueous environment."
Croatica Chemica Acta 86, 453 (2013).

L. Bytautas, N. Matsunaga, G. E. Scuseria, K. Ruedenberg
"Accurate potential energy curve for B2. 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, N. Matsunaga, K. Ruedenberg

"Accurate ab initio Potential Energy Curve of O2. II. Core-valence Correlations, Relativistic Contributions and the Vibrational-Rotation Spectrum."
Journal of Chemical Physics 132, 074307 (2010).

L. Bytautas, K. Ruedenberg
"Ab initio potential energy curve of F2. IV. Transition from the covalent to the van der Waals region: Competition between multipolar and correlation forces."
Journal of Chemical Physics 130, 204101 (2009).

L. Bytautas, K. Ruedenberg
"Correlation Energy and Dispersion Interaction in the ab initio Potential Energy Curve of the Neon Dimer."
Journal of Chemical Physics 128, 214308 (2008).

L. Bytautas, N. Matsunaga, T. Nagata, M. S. Gordon, K. Ruedenberg
"Accurate ab initio Potential Energy Curve of F2. III. The Vibration Rotation Spectrum."
Journal of Chemical Physics 127, 204313 (2007).

L. Bytautas, K. Ruedenberg
"Correlation Energy Extrapolation by Intrinsic Scaling. IV. Accurate Binding Energies of the Homonuclear Diatomic Molecules Carbon, Nitrogen, Oxygen and Fluorine."
Journal of Chemical Physics 122, 154110 (2005).

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).

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).

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).

D. J. Klein and L. Bytautas
"Graphitic Edges and Unpaired pi-electron Spins."
Journal of Physical Chemistry A 103, 5196 (1999).

L. Bytautas and D. J. Klein
"Symmetry Aspects of Nonrigid Molecules and Transition Structures in Chemical Reactions."
International Journal of Quantum Chem. 70, 205 (1998).