

## Titus V. Albu

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### EDUCATION

2000	Ph.D.	Case Western Reserve University
1995	M.S.	University of Bucharest, Romania
1994	B.S.	University of Bucharest, Romania

### PROFESSIONAL EXPERIENCE

<b>Associate Professor</b> University of Tennessee at Chattanooga, TN	2015 - present
<b>Assistant Professor</b> University of Tennessee at Chattanooga, TN	2012 - 2015
<b>Associate Professor</b> Tennessee Technological University, Cookeville, TN	2007 - 2012
<b>Visiting Research Professor</b> University of Tennessee at Chattanooga, TN	2011
<b>Assistant Professor</b> Tennessee Technological University, Cookeville, TN	2002 - 2007
<b>Postdoctoral Research Associate</b> University of Minnesota, Minneapolis, MN	2000 - 2002
<b>Graduate Assistant</b> Case Western Reserve University, Cleveland, OH	1996 - 2000
<b>Research Assistant</b> Institute of Physical Chemistry of the Romanian Academy, Bucharest, Romania	1994 - 1996
<b>Undergraduate and Graduate Assistant</b> Faculty of Chemistry, University of Bucharest, Bucharest, Romania	1989 - 1995

### HONORS AND AWARDS

- Ralph E. Powe Junior Faculty Enhancement Award, Oak Ridge Associated Universities, 2003
- Minnesota Supercomputing Institute Research Scholar Award, University of Minnesota, 2001
- Graduate Dean's Instructional Excellence Award, Case Western Reserve University, 1998
- The Department of Chemistry Award for Excellence in Graduate Student Teaching, Case Western Reserve University, 1998
- National Merit Scholarship, University of Bucharest, Bucharest, Romania, 1991-95
- 3 Mention prizes and 2 Special prizes at Chemistry National Olympiad, Romania, 1984-86

**PUBLICATIONS**

- Albu, T. V.; Patron, L.; Segal, E. "Thermal Behaviour of Some Derivatives of Malic Acid with Calcium and Strontium," *J. Thermal Anal.* **1997**, *48*, 359-366.
- Albu, T. V.; Plostinaru, S; Patron, L.; Segal, E. "Thermal Behaviour and Non-Isothermal Decomposition Kinetics of Some Nd(III) Coordination Compounds," *J. Thermal Anal.* **1997**, *50*, 425-430.
- Onutu, C.; Albu, T. V.; Segal, E.; Patron, L. "Coordination Compounds with Tarttric Acid as Ligand. I Homobinuclear Coordination Compounds of Co(II)," *Rev. Roum. Chim.* **1997**, *42*, 271-276.
- Mindru, I.; Albu, T.; Patron, L.; Segal, E.; Brezeanu, M. "Thermal Stability and Non-Isothermal Decomposition Kinetics of a Polynuclear Metal-Alkoxide Precursor of a Cobalt Ferrite," *Rev. Roum. Chim.* **1997**, *42*, 505-510.
- Albu, T. V.; Mindru, I.; Patron, L.; Segal, E.; Brezeanu, M. "Thermal behaviour of some solid coordination compounds with malic acid as ligand," *Thermochim. Acta* **1999**, *340-341*, 235-240.
- Anderson, A. B.; Albu, T. V. "Ab initio Approach to Calculating Activation Energies as Functions of the Electrode Potential. Trial Application to Four-Electron Reduction of Oxygen," *Electrochem. Comm.* **1999**, *1*, 203-206.
- Anderson, A. B.; Albu, T. V. "Ab initio Determination of Reversible Potentials and Activation Energies for Outer-Sphere Oxygen Reduction to Water and the Reverse Oxidation Reaction," *J. Am. Chem. Soc.* **1999**, *121*, 11855-11863.
- Anderson, A. B.; Albu, T. V. "Catalytic Effect of Platinum on Oxygen Reduction: An Ab Initio Model Including Dependence on the Electrode Potential," *J. Electrochem. Soc.* **2000**, *147*, 4229-4238.
- Albu, T. V.; Anderson, A. B. "Improvements to an Ab initio Model for Electrochemical Processes: Application to the Outer-Sphere Oxygen Reduction," *Electrochim. Acta* **2001**, *46*, 3001-3013.
- Albu, T. V.; Anderson, A. B.; Angus, J. C. "Dopants in Diamond Nanoparticles and Bulk. Density Functional Study of Substitutional B, N, P, SB, S, PN, O, NN, and Interstitial H," *J. Electrochem. Soc.* **2002**, *149*, E143-E147.
- Albu, T. V.; Corchado, J. C.; Truhlar, D. G. "Molecular Mechanics for Chemical Reactions: A Standard Strategy for Using Multiconfiguration Molecular Mechanics for Variational Transition State Theory with Optimized Multidimensional Tunneling," *J. Phys. Chem. A.* **2001**, *105*, 8465-8487.
- Albu, T. V.; Lynch, B. J.; Truhlar, D. G.; Goren, A.; Hrovat, D. A.; Borden, W. T.; Moss, R. A. "Dynamics of 1,2-Hydrogen Migration in Carbenes and Ring Expansion in Cyclopropylcarbenes" *J. Phys. Chem. A.* **2002**, *106*, 5323-5338.
- Zuev, P. S.; Sheridan, R. S.; Albu, T. V.; Truhlar, D. G.; Hrovat, D. A.; Borden, W. T. "Carbon Tunneling from a Single Quantum State," *Science* **2003**, *299*, 867-870.
- Albu, T. V.; Truhlar, D. G. "Force Filed Variations along the Torsional Coordinates of CH<sub>3</sub>OH and CH<sub>3</sub>CHO," *J. Molec. Spectrosc.* **2003**, *219*, 129-131.
- Lin, H.; Pu, J.; Albu, T. V.; Truhlar, D. G. "Efficient Molecular Mechanics for Chemical Reactions: Multiconfiguration Molecular Mechanics using Partial Electronic Structure Hessians," *J. Phys. Chem. A.* **2004**, *108*, 4112-4124.

- Mikel, S. E.; Albu, T. V. "Hybrid Density Functional Theory Investigation of the Hydrogen Abstraction Reaction of Fluoromethane by the Hydroxyl Radical," *J. Undergrad. Chem. Res.* **2006**, *5*, 75-81.
- Albu, T. V. "Hybrid Density Functional Theory Study of Fragment Ions Generated during Mass Spectrometry of 1,3-Dioxane Derivatives," *Rapid Commun. Mass Spectrom.* **2006**, *20*, 1871-1876.
- Albu, T. V.; Swaminathan, S. "Hybrid Density Functional Theory with Specific Reaction Parameter: Hydrogen Abstraction Reaction of Fluoromethane by the Hydroxyl Radical," *J. Phys. Chem. A.* **2006**, *110*, 7663-7671.
- De Silva, N. W. S. V. N.; Lisic, E. C.; Albu, T. V. "Hybrid Density Functional Theory Investigation of a Series of Alloxan-Based Thiosemicarbazones and Semicarbazones," *Central Eur. J. Chem.* **2006**, *4*, 646-665.
- Cai, Y.; Zhang, T.; Anderson, A. B.; Angus, J. C.; Kostadinov, L. N.; Albu, T. V. "The Origin of Shallow n-type Conductivity in Boron-Doped Diamond with H or S Co-Doping: Density Functional Theory Study," *Diam. Relat. Mater.* **2006**, *15*, 1868-1877.
- Albu, T. V.; Swaminathan, S. "Hybrid Density Functional Theory with a Specific Reaction Parameter: Hydrogen Abstraction Reaction of Trifluoromethane by the Hydroxyl Radical," *Theor. Chem. Acc.* **2007**, *117*, 383-395.
- Albu, T. V., Mikel, S. E. "Performance of Hybrid Density Functional Theory Methods toward Oxygen Electroreduction over Platinum," *Electrochim. Acta* **2007**, *52*, 3149-3159.
- De Silva, N. W. S. V. N.; Albu, T. V. "A Theoretical Investigation on the Isomerism and the NMR Properties of Thiosemicarbazones," *Central Eur. J. Chem.* **2007**, *5*, 396-419.
- Baburao, B.; Visco, D. P. Jr.; Albu, T. V. "Association Patterns in  $(\text{HF})_m(\text{H}_2\text{O})_n$  ( $m + n = 2-8$ ) Clusters," *J. Phys. Chem. A.* **2007**, *111*, 7940-7956.
- Albu, T. V.; Swaminathan, S. "Hybrid Density Functional Theory with a Specific Reaction Parameter: Hydrogen Abstraction Reaction of Difluoromethane by the Hydroxyl Radical," *J. Molec. Model.* **2007**, *13*, 1109-1121.
- Albu, T. V., Espinosa-Garcia, J.; Truhlar, D. G. "Computational Chemistry of Polyatomic Reaction Kinetics and Dynamics: The Quest for an Accurate  $\text{CH}_5$  Potential Energy Surface," *Chem. Rev.* **2007**, *107*, 5101-5132.
- Kim, J.; Vaughn, A. R.; Cho, C.; Albu, T. V.; Carver, E. A. "Modifications of Ribonuclease A Induced by p-Benzoquinone," *Bioorg. Chem.* **2012**, *40*, 92-98.
- Kim, J.; Albu, T. V.; Vaughn, A. R.; Kang, S. M.; Carver, E. A.; Stickle, D. M. "A Comparison Study on Ribonuclease A Modifications Induced by Substituted p-Benzoquinones," *Bioorg. Chem.* **2015**, *59*, 106-116.
- Hankins, M. J.; Riner, A. D., Lee, J. P.; Albu, T. V. "Synthetic, Structural and Spectroscopic Studies of Mixed Sandwich Ru(II) Complexes Involving  $\eta^6$ -p-Cymene with Monodentate Fluorine-Containing Phosphines or Phosphites," *J. Coord. Chem.* **2016**, *69*, 20-38.
- Kim, J.; Cardenal, A. D.; Greve, H. J.; Chen, W.; Vashi, H.; Grant, G.; Albu, T. V. "Interaction with calf-thymus DNA and photoinduced cleavage of pBR322 by rhodium(III) and iridium(III) complexes containing crown thioether ligands," *Inorg. Chim. Acta.* **2018**, *469*, 484-494.
- Kim, J.; Thomas, C. A.; Ewald, J. M.; Kurien, N. M.; Booker, M. E.; Greve, H. J.; Albu, T. V. "Studies on Lysozyme Modifications Induced by Substituted p-Benzoquinones," *Bioorg. Chem.* **2019**, *85*, 386-398.

## SOFTWARE DEVELOPMENT

- Zheng, J.; Bao, J. L.; Meana-Paneda, R. Zhang, S.; Lynch, B. J.; Corchado, J. C.; Chuang, Y.-Y.; Fast, P. L.; Hu, W.-P.; Liu, Y.-P.; Lynch, G. C.; Nguyen, K. A.; Jackels, C. F.; Fernandez-Ramos, A.; Ellingson, B. A.; Melissas, V. S.; Villa, J.; Rossi, I.; Coitiño, E. L.; Pu, J., Albu, T. V.; Ratkiewicz, A.; Steckler, R.; Garrett, B. C.; Isaacson, A. D.; Truhlar, D. G. POLYRATE 2017-C, Minneapolis, Minnesota, October 2018.
- Albu, T. V.; Tishchenko, O.; Corchado, C. J.; Kim, Y.; Villa, J.; Xing, J.; Lin, H.; Higashi, M.; Truhlar, D. G. MC-TINKERATE 2010, Minneapolis, Minnesota, October 2010.
- Tishchenko, O.; Higashi, M.; Albu, T. V.; Corchado, C. J.; Kim, Y.; Villa, J.; Xing, J.; Lin, H.; Truhlar, D. G. MCSI 2010, Minneapolis, Minnesota, October 2010.

## FUNDED PROJECTS

- Correlation Study of Odor Intensity and Chemico-Biological Behavior of Odorous Quinones, William H. Wheeler Research Scholar Award, University of Tennessee at Chattanooga, (2015-2016) - coPI with Dr. J. Kim
- Understanding Biological Activity of Thiosemicarbazones Using Molecular Modeling, Faculty Research Developmental Grant, Tennessee Technological University, (2012-2013)
- A Computational Study on the Nucleophilic Attack on the C=C Double Bond of Quinones, Faculty Research Development Grant, Tennessee Technological University, (2011-2012)
- An Investigation in the Biological Activity of Quinones using Fluorescence Techniques, Non-Instructional Faculty Assignment Grant, Tennessee Technological University, (2010-2011)
- Direct Dynamics Studies of Hydrogen Abstraction from Hydrofluoropropanes, Faculty Research Development Grant, Tennessee Technological University, (2008-2009)
- A Computational Study on the Reactivity of Quinones in Biological Systems, Faculty Research Development Grant, Tennessee Technological University, (2007-2008)
- A Theoretical Investigation of Hydrogen Abstraction from Hydrohalocarbons, Faculty Research Grant, Tennessee Technological University, (2005-2006)
- Theoretical Investigation of Oxygen Electroreduction over Platinum, Faculty Research Grant, Tennessee Technological University, (2004-2005)
- Theoretical Study of the Electrochemical Processes in Fuel Cells, Ralph E. Powe Junior Faculty Enhancement Award, Oak Ridge Associated Universities (2003-2004)

## DIRECTED THESIS

- Nuwan De Silva “Theoretical Studies of Thiosemicarbazones and Hydrofluorocarbons,” MS Thesis, Tennessee Technological University, **2007**
- Roshan Fernando “Theoretical Studies on Quinone Reactivity,” MS Thesis, Tennessee Technological University, **2009**
- Wasana Senevirathna “Theoretical Studies of Hydrogen Abstraction from Hydrofluoropropanes,” MS Thesis, Tennessee Technological University, **2009**
- Lasantha Rathnayake “Theoretical Investigations of p-Benzoquinones and Thiosemicarbazones,” MS Thesis, Tennessee Technological University, **2013**
- Charles A. Thomas “Fluorescence and UV-Vis Studies of Quinone-Induced Protein Modifications,” Departmental Thesis, University of Tennessee at Chattanooga, **2017**

**TEACHING EXPERIENCE**

General Chemistry I (lecture and lab)

General Chemistry II (lecture and lab)

General Chemistry I Honors Recitation

General Chemistry II Honors Recitation

Organic Chemistry I (lecture and lab) – as a substitute

Chemistry Literature

Chemistry Seminar

Elements of Physical Chemistry

Physical Chemistry I (lecture and lab)

Physical Chemistry II (lecture and lab)

Advanced Physical Chemistry – Physical Organic Chemistry

Advanced Physical Chemistry – Computational Chemistry

Special Topics – Molecular Modeling

Special Topics – Computational Chemical Dynamics