VASILIOS STERGIOU MELISSAS

Section of Physical Chemistry

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PLACE AND DATE OF BIRTH

Thessaloniki, Greece 1 August 1963

CITIZENSHIP

Greek

MARITAL STATUS

Married

MILITARY STATUS

Military service completed 21 September 1993–21 September 1994

EDUCATION

Ph.D., Chemistry August 1993

University of Minnesota, Minneapolis, Minnesota, USA

Thesis: Improved Methods for the Calculation of Minimum Energy Paths in Chemical Dynamics and Reaction Rates Calculation for Reactions of OH with Alkanes

Adviser: Dr. Donald G. Truhlar

B.Sc., Chemistry October 1986

Aristotle University of Thessaloniki, Thessaloniki, Greece

LANGUAGES

English–Excellent

French–Very well

VASILIOS STERGIOU MELISSAS

RESEARCH EXPERIENCE

Associate Professor — 16 July 2012
University of Ioannina
School of Natural Sciences
Department of Chemistry
Section of Physical Chemistry

Assistant Professor — 11 April 2006–16 July 2012
University of Ioannina
School of Natural Sciences
Department of Chemistry
Section of Physical Chemistry

Lecturer — 20 June 2001–11 April 2006
University of Ioannina
School of Natural Sciences
Department of Chemistry
Section of Physical Chemistry

Adjunct Assistant Professor — 1 September 2000–20 June 2001
University of Ioannina
School of Natural Sciences
Department of Materials Science & Engineering

Associate Researcher D´ — 1 October 1997–20 June 2001
N.R.C.P.S. “Demokritos”
Institute of Physical Chemistry
Molecular Modeling of Materials Laboratory

Postdoctoral Fellow — 1 September 1995–30 September 1997
Aristotle University of Thessaloniki
Department of Chemistry
Laboratory of Applied Quantum Chemistry

Research Assistant — 23 March 1994–21 September 1994
Greek Army

VASILIOS STERGIOU MELISSAS

Graduate Fellow-Research/Teaching Assistant 16 March 1987–15 June 1993
University of Minnesota
Department of Chemistry

DEGREES AWARDED AND UNDER PREPARATION

Two (2) Ph.D. degrees awarded, two (2) under preparation.
Four (4) Master's degrees awarded, one (1) under preparation.

RESEARCH INTERESTS

- Atmospheric chemistry
- Theoretical investigation of important mechanisms in biochemistry
- Applications of Variational Transition State Theory with multidimensional semiclassical tunneling contributions
- Development of potential energy functions and classical force fields, suitable for molecular simulations exploration

SELECTED PUBLICATIONS

- "Rotation of Methyl Groups in Hexamethylbenzene," V. Melissas, K. Fægri, and J. Almlöf. J. Am. Chem. Soc. **107**, 4640 (1985).
- "Optimized Calculations of Reaction Paths and Reaction-Path Functions for Chemical Reactions," V. S. Melissas, D. G. Truhlar and B. C. Garrett, J. Chem. Phys. **96**, 5758 (1992).
- "POLYRATE 4: A New Version of a Computer Program for the Calculation of Chemical Reaction Rates for Polyatomics," D.-h. Lu, T. N. Truong, V. S. Melissas, G. C. Lynch, Y.-P. Liu, B. C. Garrett, R. Steckler, A. D. Isaacson, S. N. Rai, G. C. Hancock, J. G. Lauderdale, T. Joseph and D. G. Truhlar, Comput. Phys. Commun. **71**, 235 (1992).
- "MORATE: A Program for Direct Dynamics Calculations of Chemical Reaction Rates by Semiempirical Molecular Orbital Theory," T. N. Truong, D.-h. Lu, G. C. Lynch, Y.-P. Liu, V. S. Melissas, J. J. P. Stewart, R. Steckler, B. C. Garrett, A. D. Isaacson, A. Gonzalez-Lafont, S. N. Rai, G. C. Hancock, T. Joseph, and D. G. Truhlar, Comput. Phys. Commun. **75**, 143 (1993).
- "Interpolated Variational Transition State Theory and Tunnelling Calculations of the Rate Constant of the Reaction OH + CH_4 at 223–2400 K," V. S. Melissas and D. G. Truhlar, J. Chem. Phys. **99**, 1013 (1993).
- "Deuterium and Carbon-13 Kinetic Isotope Effects for the Reaction of OH with CH_4," V. S. Melissas and D. G. Truhlar, J. Chem. Phys. **99**, 3542 (1993).
- "Interpolated Variational Transition State Theory and Semiclassical Tunnelling Calculations of the Rate Constant of the Reaction OH + C_2H_6," V. S. Melissas and D. G. Truhlar, J. Phys. Chem. **98**, 875 (1994).
- "POLYRATE 6.5: A New Version of a Computer Program for the Calculation of Chemical Reaction Rates for Polyatomics," R. Steckler, W.-P. Hu, Y.-P. Liu, G. C. Lynch, B. C. Garrett, A. D. Isaacson, V.

S. Melissas, D.-h. Lu, T. N. Truong, S. N. Rai, G. C. Hancock, J. G. Lauderdale, T. Joseph and D. G. Truhlar, Comput. Phys. Commun. **88**, 341 (1995).

- "MORATE 6.5: A New Version of a Computer Program for Direct Dynamics Calculations of Chemical Reaction Rate Constants," W.-P. Hu, G. C. Lynch, Y.-P. Liu, I. Rossi, J. J. P. Stewart, R. Steckler, B. C. Garrett, A. D. Isaacson, D.-h. Lu, V. S. Melissas and D. G. Truhlar, Comput. Phys. Commun. **88**, 344 (1995).
- "*Ab Initio* Calculations for $(BrO)_2$ System and Quasiclassical Dynamics Study of BrO Self-Reaction," D. Papayannis, A. M. Kosmas and V. S. Melissas, Chem. Phys. **243**, 249 (1999).
- "Dynamics of the OH + Cl_2 → HOCl + Cl Reaction: *Ab Initio* Investigation and Quasiclassical Trajectory Calculations of Reaction Selectivity," V. S. Melissas, E. Drougas, E. G. Bakalbassis and A. M. Kosmas, J. Phys. Chem. A **104**, 626 (2000).
- "Quantum Mechanical Studies on the BrO + ClO Reaction," D. K. Papayannis, A. M. Kosmas and V. S. Melissas, J. Phys. Chem. A **105**, 2209 (2001).
- "*Ab Initio* and Density Functional Theory Studies for the Explanation of the Antioxidant Activity of Certain Phenolic Acids," E. G. Bakalbassis, A. Chatzopoulou, V. S. Melissas, M. Tsimidou, M. Tsolaki and A. Vafiadis, Lipids **36**, 181 (2001).
- "A Quantum Mechanical Study of the Structure, Vibrational Spectra, and Relative Energetics of XOOI, XIO_2, and XOIO (X = Cl, Br, and I) Isomers," D. K. Papayannis, V. S. Melissas and A. M. Kosmas, Chem. Phys. Lett. **349**, 299 (2001).
- "A Quantum Mechanical Study of IOX (X = Cl, Br, I) Isomers," D. K. Papayannis, V. S. Melissas and A. M. Kosmas, Chem. Phys. Lett. **363**, 99 (2002).
- "Structural and Relative Stability Studies of IOOX Peroxides (X = Cl, Br, I) and their Isomers," V. S. Melissas, D. K. Papayannis and A. M. Kosmas, J. Mol. Struc.-Theochem **626**, 263 (2003).
- "Quantum Mechanical Studies of Methyl Bromoperoxide Isomers and the CH_3O + BrO Reaction," D. K. Papayannis, V. S. Melissas and A. M. Kosmas, Phys. Chem. Chem. Phys. **5**, 2976 (2003).
- "An Extremely Stable Ni(II) Complex Derived from the Hydrolytic Cleavage of the C-Terminal Tail of Histone H2A," M. Mylonas, J. C. Plakatouras, N. Hadjiliadis, K. D. Papavasileiou and V. S. Melissas, J. Inorg. Biochem. **99**, 637 (2005).
- "Molecular Simulation of Structure, Thermodynamic and Transport Properties of Polymeric Membrane Materials for Hydrocarbon Separation," I. G. Economou, V. E. Raptis, V. S. Melissas, D. N. Theodorou, J. Petrou and J. H. Petropoulos, Fluid Phase Equilibr. **228–229**, 15 (2005).
- "An *Ab Initio* Study of the Kinetics of the CH_3Cl + OH Reaction," T. D. Tzima, D. Papayannis and V. S. Melissas, Chem. Phys. **312**, 169 (2005).
- "Theoretical kinetic study of the CH_3Br + OH atmospheric system," T. D. Tzima, K. D. Papavasileiou, D. K. Papayannis and V. S. Melissas, Chem. Phys. **324**, 591 (2006).
- "The photo-Fries rearrangement of 9-Trimethylsilyl Substituted Xanthenes," M. G. Siskos, A. K. Zarkadis, P. S. Gritzapis, O. Brede, R. Hermann, V. S. Melissas, G. G. Gurzadyan, A. S. Triantafyllou and V. Georgakilas, J. Photoch. Photobio. A **182**, 17 (2006).

- "Force Field Development for Poly(dimethylsilylenemethylene) with the Aid of *Ab Initio* Calculations," V. E. Raptis and V. S. Melissas, J. Phys. Chem. B **110**, 14929 (2006).
- "Resonance-Enhanced Multiphoton Ionization of Jet-Cooled 2-Methylfuran," J. G. Philis and V. S. Melissas, Chem. Phys. **336**, 136 (2007).
- "An experimental and theoretical study of the $S_1 \leftarrow S_0$ Transition of *p*Ethynyltoluene," J. G. Philis and V. S. Melissas, J. Chem. Phys. **127**, 204310 (2007).
- "A DFT Study of the Nitric Oxide and Tyrosyl Radical Interaction: A Proposed Radical Mechanism," K. D. Papavasileiou, T. D. Tzima, Y. Sanakis and V. S. Melissas, ChemPhysChem **8**, 2595 (2007).
- "Multifrequency Electron Paramagnetic Spectroscopic and Theoretical Studies of a Mn(II) (S = 5/2) complex. The role of geometrical elements on the Zero Field Splitting Parameters," T. D. Tzima, G. Sioros, D. Kovala-Demertzi, V. S. Melissas and Y. Sanakis, Polyhedron **28**, 3257 (2009).
- "A two-Dimensional Magnetic Hybrid Material based on Intercalation of a Cationic Prussian blue analogue in Montmorillonite Nanoclay," D. Gournis, C. Papachristodoulou, E. Maccallini, P. Rudolf, M. A. Karakassides, D. T. Karamanis, M.-H. Sage, T. T. M. Palstra, J.-F. Colomer, K. D. Papavasileiou, V. S. Melissas and N. H. Gangas, J. Colloid Interf. Sci. **348**, 393 (2010).
- "A "hidden" role of amino and imino groups is unveiled during the micro-solvation study of three biomolecule groups in water," P. G. Takis, V. S. Melissas and A. N. Troganis, New J. Chem. **36**, 1866 (2012).
- "Electronic and magnetic properties of the binuclear $[Mn_2\{(OPPh_2)_2N\}_4]$ complex, as revealed by magnetometry, EPR and density functional broken-symmetry studies," T. D. Tzima, E. Ferentinos, D. Maganas, V. S. Melissas, Y. Sanakis and P. Kyritsis, Polyhedron **52**, 706 (2013).
- "Probing microsolvation in "numbers": the case of neutral dipeptides in water," P. G. Takis, K. D. Papavasileiou, L. D. Peristeras, V. S. Melissas and A. N. Troganis, Phys. Chem. Chem. Phys. **15**, 7354 (2013).

BOOK CHAPTERS

- P. G. Takis, K. D. Papavasileiou, A. N. Troganis and V. S. Melissas, in *Betaine*, edited by V. R. Preedy (Royal Society of Chemistry, Cambridge, 2014), pp. XX–XX.
- P. G. Takis, K. D. Papavasileiou, A. N. Troganis and V. S. Melissas, in *Betaine*, edited by V. R. Preedy (Royal Society of Chemistry, Cambridge, 2014), pp. XX–XX.