**Curriculum Vitae**

# Nicholas Dominick Koslap Petraco

Assistant Professor of Chemistry

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## Educational Background:

University of Waterloo — Post-doctoral Fellowship — September 2002 - August 2004
Faculty of Mathematics
Dept. of Applied Mathematics
Waterloo, Ontario, Canada

Post doctoral research under the direction of Prof. Josef Paldus involved the diagrammatic formulation of generalized Hilbert space multireference coupled cluster theory to compute physical properties for excited states of medium sized molecules. Also, a new group theoretical approach was developed for the evaluation of arbitrary spin-symmetry-adapted matrix elements arising in configuration interaction and coupled cluster quantum chemical computations.

University of Georgia — Ph.D. Theoretical Chemistry — July 1998 - May 2002
Center for Computational
Quantum Chemistry
Athens, Georgia

Graduate research under the direction of Prof. Henry F. Schaefer involved investigation of the intruder state problem in perturbation and coupled cluster theories of electronic structure, as well as the prediction of fragmentation pathways, hyperfine coupling constants and molecular properties of small and medium sized organic compounds using *ab initio* electronic structure theory.

Colgate University — A.B. Chemistry — August 1994 - May 1998
Hamilton, New York — (*Magna Cum Laude*)

Undergraduate research under the direction of Prof. John C. Cochran included the synthesis, characterization and theoretical analysis of organo-tin complexes.

## Professional Experience:

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| Assistant Professor of Chemistry | Department of Science<br>City University of New York<br>John Jay College<br>and Faculty of Chemistry<br>The Graduate Center of CUNY<br>New York, New York | September 2004 - Present |

Currently teaching physical chemistry I (classical equilibrium thermodynamics), physical chemistry II (quantum mechanics and theoretical spectroscopy), computational quantum chemistry and general introductory chemistry. Also conducting research into the mechanisms of ninhydrin amino acid reactions, application of group representation theory to quantum chemistry and construction of databases of toolmark impression characteristics for use in statistical comparisons.

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| Calculus 1 Instructor | Faculty of Mathematics<br>Department of Applied Mathematics<br>University of Waterloo<br>Waterloo, Ontario, Canada | September 2003 - December 2003 |

Delivered lectures, graded and tutored introductory calculus for scientists and engineers.

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| Teaching Assistant | Center for Computational<br>Quantum Chemistry and<br>Department of Chemistry<br>University of Georgia<br>Athens, Georgia | January 2002 - April 2002 |

Graded and tutored graduate level advanced molecular quantum mechanics course. In addition, delivered course lectures pertaining to second quantization, diagrammatic techniques and non variational methods of electron correlation.

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| Summer Program Lecturer<br>and Mentor | Center for Computational<br>Quantum Chemistry<br>University of Georgia<br>Athens, Georgia | June 2000 - August 2002 |

Lectured on molecular quantum mechanics each summer to undergraduates and first-year graduate students. Topics included configuration interaction theory, second quantization, diagrammatic techniques, perturbation theory and coupled cluster theory. Served as mentor to students on applications oriented quantum chemistry research projects.

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| Teaching Assistant | Department of Chemistry<br>University of Georgia<br>Athens, Georgia | August 1998 - May 2000 |

Taught general chemistry laboratory sections, tutored general and organic chemistry students.

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| Summer Research Assistant | Department of Chemistry<br>Colgate University<br>Hamilton, New York | June 1996 - August 1996 and<br>June 1997 - August 1997 |

Characterized the reaction between phenylacetylene and trialkyl substituted tin hydrides using both experimental and semi-empirical theoretical techniques.

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| Teaching Assistant | Department of Chemistry<br>Colgate University<br>Hamilton, New York | August 1995 - May 1997 |

Provided laboratory instruction for general and organic chemistry.

## Grants:

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| PSC-CUNY Research Award | $4,800 |
| PSC-CUNY Research Award | $2,900 |
| RF-CUNY Start-up Award | $30,000 |

## Academic Honors:

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| International Cooperative Agreement Between Comenius University and The University of Georgia Recipient | Comenius University<br>Bratislava, Slovakia<br>University of Georgia<br>Athens, Georgia | November 2001 and<br>September 2002 |

## Publications:

### Journal Articles:

1. Yukio Yamaguchi, Nicholas D. K. Petraco, Shawn T. Brown, and Henry F. Schaefer III, "The 1-Silaketenyl Radical (HSiCO): Ground and First Excited Electronic States," *J. Chem. Phys.* **112**, 2168 (2000).

2. Nicholas D. K. Petraco, Shawn T. Brown, Yukio Yamaguchi and Henry F. Schaefer III, "The Silaketenylidene (SiCO) Molecule: Characterization of the $\tilde{X}\ ^3\Sigma^-$ and $\tilde{A}\ ^3\Pi$ States," *J. Chem. Phys.* **112**, 3201 (2000).

3. Nicholas D. K. Petraco, Steven S. Wesolowski, Matthew L. Leininger and Henry F. Schaefer III, "Coupled-Cluster Studies of the Hyperfine Splitting Constants of the Thioformyl Radical," *J. Chem. Phys.* **112**, 6245 (2000).

4. Nicholas D. K. Petraco, Shawn T. Brown, Yukio Yamaguchi and Henry F. Schaefer III, "The 2-Silaketenylidene (CSiO) Radical: Electronic Structure of the $\tilde{X}\ ^3\Sigma^-$ and $\tilde{A}\ ^3\Pi$ States," *J. Phys. Chem. A* **104**, 10165 (2000).

5. Yukio Yamaguchi, Shawn T. Brown, Nicholas D. K. Petraco and Henry F. Schaefer III, "The 2-Silaketenyl Radical (HCSiO): Ground and First Excited Electronic States," *J. Mol. Struct.* **556**, 293 (2000).

6. Nicholas D. K. Petraco, David A. Modarelli and John C. Cochran, "The Structure of the Intermediate Radical in the Hydrostannation of Phenylacetylene," *Syn. React. Inorg. Met.* **31**, 757 (2001).

7. Shawn T. Brown, Nicholas D. K. Petraco, Yukio Yamaguchi, and Henry F. Schaefer III, "$\tilde{X}\ ^3\Sigma^-$ and $\tilde{A}\ ^3\Pi$ Electronic States of Disilaketenylidene (SiSiO): Analysis of the Renner Effect. Comparison with the Analogous Multiple Bonded Systems SiCO, CSiO, and CCO," *Polyhedron* **21**, 599 (2002).

8. Ľuboš Horný, Nicholas D. K. Petraco, Chaeho Pak and Henry F. Schaefer III, "What is the Nature of Polyacetylene Neutral and Anionic Chains $HC_{2n}H$ and $HC_{2n}H^-$ that have recently been observed?" *J. Am. Chem. Soc.* **124**, 5861 (2002).

9. Nicholas D. K. Petraco, Wesley D. Allen and Henry F. Schaefer III, "The Fragmentation Path for Hydrogen Dissociation from Methoxy Radical," *J. Chem. Phys.* **116**, 10229 (2002).

10. John C. Cochran, V. Prindle, H. A. Young, M. H. Kumar, S. Tom, Nicholas D. K. Petraco, C. Mohoro and B. Kelley, "Alkyl- and acyl-substituted vinylstannanes: Synthesis and reactivity in electrophilic substitution reactions," *Syn. React. Inorg. Met.* **32**, 885 (2002).

11. Nicholas D. K. Petraco, Ľuboš Horný, Henry F. Schaefer III and Ivan Hubač, "Brillouin-Wigner Coupled Cluster Theory: Fock-Space Approach," *J. Chem. Phys.* **117**, 9580 (2002).

12. Ľuboš Horný, Nicholas D. K. Petraco and Henry F. Schaefer III, "Odd carbon long linear chains $HC_{2n+1}H$ (n=4-11): Properties of the neutrals and radical anions," *J. Am. Chem. Soc.* **124**, 14716 (2002).

13. Josef Paldus, Xiangzhu Li and Nicholas D. K. Petraco, "General-Model-Space State-Universal Coupled Cluster Method: Diagrammatic Approach," *J. Math. Chem.* **35**, 215 (2004).

14. Nicholas Petraco, Nicholas D. Petraco, Peter A. Pizzola, "An Ideal Material for the Preparation of Known Toolmark Test Impressions," *J. Forensic Sci.* **50**, 1407 (2005).

15. Nicholas D. Petraco, Gloria Proni, Jennifer J. Jackiw and Anne-Marie Sapse, "Amino acid alanine reactivity with the fingerprint reagent ninhydrin. A detailed ab-initio computational study," *J. Forensic Sci.* **51**, 1267 (2006)

16. Nicholas D. Petraco, "Easy Spin-Symmetry-Adaptation. Exploiting the Clifford Algebra Unitary Group. Derivation of Working Equations for Arbitrary Time-Independent Spin-Adapted Matrix Elements," *Proceedings of the* $26^{th}$ *International Colloquium on Group Theoretical Methods in Physics* (2007)

17. Christopher Yung-Fou Chen, Nicholas D. K. Petraco, Christopher J. Barden and Jeffrey Cheng-Lung Lee, "An Electron Correlated Examination of the Reactivity of Fingerprint Reagent Ninhydrin" *Proceedings of the Taiwanese Academy of Forensic Science* (2007)

18. Danielle Sapse and Nicholas D. Petraco, "Substituted ninhydrin and Ruhemann's Purple derivatives. Reaction energetics and comments on consequences for the law," J. Mol. Modeling **13**, 943 (2007)

19. Nicholas D. K. Petraco, Mark Gil, Peter A. Pizzola and Thomas A. Kubic, "Statistical Discrimination of Several Gasoline Samples From Casework," *J. Forensic Sci.* (2008) *Accepted.*

20. Nicholas Petraco, Thomas A. Kubic and Nicholas D. K. Petraco, "Case Studies in Forensic Soil Examinations," *Forensic Sci. International Accepted.*

21. Nicholas Petraco, Nicholas D. K. Petraco, Lisa Faber, and Peter A. Pizzola, "Preparation of Tool Mark Standards with Jewelry Modeling Waxes," *J. Forensic Sci.* (2008) *Accepted.*

## Submitted:

1. Nicholas D. K. Petraco, Carol Gambino, Thomas A. Kubic, Dayhana Olivo and Nicholas Petraco, "Statistical Discrimination of Footwear: A method for the comparison of accidentals on shoe outsoles inspired by facial recognition techniques," *Submitted.*

## In Preparation:

1. Nicholas D. K. Petraco "How Statistical Pattern Comparison Methods can be Applied to Toolmarks" *In Preparation.*

2. Nicholas D. K. Petraco and Josef Paldus, "A Pedagogical Introduction to Unitary Group Representation Theory and Its Applications in Quantum Chemistry," *In Preparation.*

## In Progress:

1. "Time Series Statistical Analysis of Accidental Patterns on the Soles of Shoes"

2. "Fingerprinting of Station Gasoline using Gas Chromatography-Flame Ionization Detection (GC-FID) and Statistical Pattern Recognition"

## Scientific Presentations:

1. Poster: "Coupled-Cluster Studies of the Hyperfine Splitting Constants of the Thioformyl Radical," 28th Southeastern Theoretical Chemistry Association Conference, University of Memphis, Memphis, Tennessee, April 22 1999.

2. Poster: "The Silaketenylidene (SiCO) Molecule: Characterization of the $\tilde{X}\ ^3\Sigma^-$ and $\tilde{A}\ ^3\Pi$ States," 5th Triennial Meeting of the World Association of Theoretically Oriented Chemists, Imperial College, London, England, August 2 1999.

3. Poster: "The 2-Silaketenylidene (CSiO) Radical: Electronic Structure of the $\tilde{X}\ ^3\Sigma^-$ and $\tilde{A}\ ^3\Pi$ States," 29th Southeastern Theoretical Chemistry Association Conference, University of Georgia, Athens, Georgia, May 20 2000.

4. Poster: "The Fragmentation Path for Hydrogen Dissociation from Methoxy Radical," Molecular Quantum Mechanics: The Right Answer for the Right Reason, An International Conference in Honor of Ernest R. Davidson, University of Washington, Seattle, Washington, July 22 2001.

5. Lecture: "The Fragmentation Path for Hydrogen Dissociation from Methoxy Radical," University of Waterloo, Waterloo, Canada, December 14 2001.

6. Poster: "Brillouin-Wigner Coupled Cluster Theory: Fock-Space Approach," 6th Triennial Meeting of the World Association of Theoretically Oriented Chemists, Locarno, Switzerland, August 2 2002.

7. Lecture: "Amino acid alanine reactivity with the fingerprint reagent ninhydrin. A detailed ab-initio computational study," University of Rouen, Rouen, France, June 26 2006.

8. Lecture: "Easy Spin-Symmetry-Adaptation. Exploiting the Clifford Algebra Unitary Group. Derivation of Working Equations for Arbitrary Time-Independent Spin-Adapted Matrix Elements," 26th International Colloquium on Group Theoretical Methods in Physics, New York, New York, June 29 2006.

9. Lecture: "What Quantum Chemistry Can Do for Forensic Science," Department of Chemistry, Brooklyn College, New York, New York, September 1, 2006.

10. Lecture: "An Electron Correlated Examination of the Reactivity of Fingerprint Reagent Ninhydrin," 2006 National Meeting of the Taiwanese Academy of Forensic Science, Taipei, Taiwan, November 10, 2006.

11. Lecture: "Algebraic Symmetries in Quantum Chemistry: Clifford Algebra and Para-Fermi Algebra in Correlated Many-Electron Theories". Department of Chemistry, Queens College, New York, New York, March 26, 2007.

12. Poster: "Statistical Discrimination of Footwear: A method for the comparison of accidentals on shoe outsoles inspired by facial recognition techniques". North Eastern Association of Forensic Scientists $33^{rd}$ Annual Meeting, Bolton Landing, New York, October 31, 2007.

13. Lecture: "Statistical Discrimination of Gasoline Samples From Casework". American Academy of Forensic Science Annual Meeting, Washington D. C., February 18, 2008.