SHORT CURRICULUM VITAE

JANE S. MURRAY

PERSONAL DATA:

Date and Place of Birth: August 23, 1955; San Rafael, California, USA
Citizenship: USA

EDUCATION:

Undergraduate:	Temple University, 1973-1975.
	Miami University (Ohio), 1976-1978; B.S. Chemistry, 1978.
Graduate:	University of Georgia, 1978-1979.
	University of New Orleans; Ph.D. Physical Chemistry, 1986.

DISSERTATION TITLE: Computational Studies in Chemical Toxicology.

PROFESSIONAL POSITIONS:

Analytical Chemistry Intern, Procter & Gamble Co., Paper Products Division, Cincinnati, Ohio, Summer 1979.

Chemist, Thionville Laboratories, Inc., Elmwood Industrial Park, New Orleans, LA, September 1979 - December 1979.

Laboratory Manager, Thionville Laboratories, Inc. Elmwood Industrial Park, New Orleans, LA June 1987 - September 1988.

Editor, LSU Eye Center, Dept of Ophthalmology, LSU Medical Center, New Orleans, LA, October 1988 - February 1989.

Research Associate in Theoretical Chemistry, University of New Orleans, New Orleans, LA, February 1989 - March 1994.

Assistant Professor - Research, University of New Orleans, New Orleans, LA, March 1994 - 2006.

Senior Research Associate, Department of Chemistry, University of New Orleans, December 2007 – August 2023.

Professor Emeritus, Department of Chemistry, University of New Orleans, September 2023 – present.

PROFESSIONAL ACTIVITIES:

(1) Treasurer, International Society of Quantum Biology and Pharmacology, 1999 – 2007.
(2) Executive Board, Environment and Health Council of Louisiana, 2000 – present.

(3) Chair, 2005-2006, Louisiana Section of the ACS; Chair-Elect, 2004; Secretary, 2003; recipient of an ACS Local Section Innovative Projects Grant Proposal in 2004 for organizing a workshop addressing the topic: "Chemical Manufacturing in Louisiana: What are our Options?"
(4) Secretary, University of New Orleans Chapter, Sigma Xi, The Scientific Research Society, 1989-2007.
(5) Co-organizer, Computational Chemistry Symposium, CERMACS Meeting, Cleveland, OH, May 2009.
(6) Co-organizer, Computational/Experimental Characterization of Advanced Materials, SE/SW ACS Meeting, New Orleans, LA, December 2010.
(7) Associate Editor, J. Molecular Modeling, 2015-present.

INVITED SPEAKER IN MEETINGS AND SYMPOSIA:

1. Gordon Conference on Electron Densities, Plymouth, NH, July 1992.
2. First Southern School of Computational Chemistry, Orange Beach, AL, March 2001 (invited speaker).
3. Modelling and Design of Molecular Materials Workshop, Wroclaw, Poland, September 2004 (invited speaker).
4. Fifth Southern School of Computational Chemistry, Jackson, MS, April 2005 (invited speaker).
5. Modeling Interactions in Biomolecules Workshop-II, Prague, Czech Republic, September 2005 (invited speaker).
6. Sixth Southern School of Computational Chemistry, Jackson, MS, March 2006 (invited speaker).
7. Mini-Symposium in Theoretical and Computational Chemistry, Santiago, Chile, January 2007 (invited speaker).
8. Methods and Applications in Computational Chemistry-2 (MACC-2), Kiev, Ukraine, July 2007 (invited speaker).
9. Conference on Modeling Interactions in Biomolecules-III (MIB-III), Prague, Czech Republic, September 2007 (invited speaker).
10. Modelling and Design of Molecular Materials Conference 2008, Piechowice, Poland, June 2008 (invited speaker).
11. Sixth Southern School of Computational Chemistry and Materials Science, Jackson, MS, July 2009 (invited speaker).
12. Conference on Modeling Interactions in Biomolecules-III (MIB-III), Hruba Skala, Czech Republic, September 2009 (invited speaker).
13. Mini-Symposium: Summer Talks in Santiago, Santiago, Chile, January 2010 (invited speaker).
14. Modelling and Design of Molecular Materials Conference 2010, Wroclaw, Poland, July 2010 (invited speaker).
15. Summer Talks in Santiago III (Politzer Conference), January 2012 (invited speaker).
16. Gordon Research Conference on Crystal Engineering, Waterville Valley, NH, June 2012 (invited speaker).
17. Modelling and Design of Molecular Materials Conference 2012, Wroclaw, Poland, September 2012 (invited speaker).
18. Virtual Conference in Computational Chemistry (VCCC-2013), University of Mauritius, Mauritius, August 2013 (invited presentation).

19. Conference on Modeling Interactions in Biomolecules-VI (MIB-VI), Marianske Lazne, Czech Republic, September 2013 (invited speaker).
20. Conference on Current Trends in Computational Chemistry (CCTCC), Jackson, MS, November 2013 (invited speaker).
21. Modelling and Design of Molecular Materials Conference 2014, Kudowa Zdroj, Poland, July 2014 (invited speaker).
22. Virtual Conference in Computational Chemistry (VCCC-2014), University of Mauritius, Mauritius, August 2014 (invited presentation).
23. Winter School in Computational Chemistry, February 2015 (invited presentation).
24. Virtual Conference in Computational Chemistry (VCCC-2015), University of Mauritius, Mauritius, August 2015 (invited presentation).
25. Conference on Modeling Interactions in Biomolecules-VII (MIB-VII), Praha-Průhonice, Czech Republic, September 2015 (invited speaker).
26. Sanibel Symposium, Saint Simons Island, GA, February 2016 (invited speaker).
27. Conference on Current Trends in Computational Chemistry (CCTCC), Jackson, MS, November 2016 (invited speaker for joint talk with Peter Politzer).
28. International Symposium on Halogen Bonding (ISXB3), Greenville, SC, June 2018 (invited speaker).
29. Conference on Current Trends in Computational Chemistry (CCTCC), Jackson, MS, November 2019 (invited speaker).
30. Conference on Modeling Interactions in Biomolecules-IX (MIB-2023), Praha-Průhonice, Czechia, September 2023 (invited speaker).
31. International Conference on Noncovalent Interactions-III (ICNI-III), Belgrade, Serbia, June 2024 (invited speaker).
32. Conference on Current Trends in Theoretical Chemistry – IX, Krakow, Poland, September 2024 (invited speaker).

INVITED LECTURES: 11 total, the last being at the University of Colorado Denver, Denver, CO, October 2023.

SCIENTIFIC PUBLICATIONS: Total: 347, included below are papers from 2020 onward:

(307) "Hydrogen Bonding – A Coulombic σ-Hole Interaction"
Jane S. Murray and P. Politzer, J. Ind. Inst. Sci., 100, 21-30 (2020).

(308) Electrostatics and Polarization in σ- and π-Hole Noncovalent Interactions: An Overview"
P. Politzer and J. S. Murray, ChemPhysChem, 21, 579-588 (2020).

(309) "Interaction and Polarization Energy Relationships in σ-Hole and π-Hole Bonding"
J. S. Murray and P. Politzer, Crystals, 10, 76(1-18) (2020).

(310) ""Conformation Pinning" by Anion Attachment Enabling Separation of Isomeric Steroid Monomers by Ion Mobility Spectrometry"
R. B. Cole, C. Albers, P. Bayat and J. S. Murray, J. Mass Spectrom., 55, e4657(1-11) (2020).

(311) "Oxatriazoles: Potential Frameworks for Energetic Compounds?"
P. Politzer and J. S. Murray, Propell. Explos. Pyrotech. 46, 222-232 (2021).

(312) "Electrostatic Potentials at the Nuclei of Atoms and Molecules"
P. Politzer and J. S. Murray, Theor. Chem. Accts., 140, 7 (2021).

(313) "Tetrel and Pnictogen Bonds Complement Hydrogen and Halogen Bonds in Framing the Interactional Landscape of Barbituric Acids"
K. Vijit, P. Scilabra, P. Politzer, G. Terraneo, A. Daolio, F. Fernandez-Palacio, J. S. Murray and G. Resnati, Cryst. Growth Des., 21, 642-652 (2021).

(314) "The Use and Misuse of van der Waals Radii"
P. Politzer and J. S. Murray, Struct. Chem. 32, 623-629 (2021); DOI: 10.1007/s11224-020-01713-7.

(315) "The Many Faces of Fluorine: Some Noncovalent Interactions of Fluorine Compounds"
J. S. Murray, P. G. Seybold and P. Politzer, J. Chem. Thermodyn. 156, 106382(1-11) (2021).

(316) "Molecular Electrostatic Potentials: Significance and Applications"
P. Politzer and J. S. Murray, in Chemical Reactivity in Confined Systems: Theory, Modelling and Applications, P. K. Chattaraj and D. Chakraborty, eds., John Wiley, Oxford, UK, 2021, ch. 7, pp. 113-134.

(317) "Some Molecular and Crystalline Factors that Affect the Sensitivities of Explosives"
P. Politzer and J. S. Murray, in NAME OF VOLUME, D. Mathieu, ed., *Theoretical and Computational Chemistry*, Elsevier, Amsterdam, 2021, in press.

(318) "Identifying the Most Energetic Electrons in a Molecule: The Highest Occupied Molecular Orbital and the Average Local Ionization Energy"
F. A. Bulat, J. S. Murray and P. Politzer, Comput. Theoret. Chem., 1199, 113192 (2021).

(319) "Can Counter-Intuitive Halogen Bonding be Coulombic?"
J. S. Murray and P. Politzer, ChemPhysChem, 22. 1201-1207 (2021).

(320) "The Neglected Nuclei"
P. Politzer and J. S. Murray, Molecules, 26, 2982 (2021).

(321) "The π-Hole Revisited"
P. Politzer, J. S. Murray and T. Clark, Phys. Chem. Chem. Phys., 23, 16458-16468 (2021).

(322) "Are HOMO-LUMO Gaps Reliable Indicators of Explosive Impact Sensitivity?"
P. Politzer and J. S. Murray, J. Mol. Model., 27, 327 (2021).

(323) "The Conceptual Power of the Hellmann-Feynman Theorem"
P. Politzer and J. S. Murray, Struct. Chem., 34, 17-21 (2023).

(324) "Interpreting the Variations in the Kinetic and Potential Energies in the Formation of a Covalent Bond"
T. Clark, P. Politzer and J. S. Murray, Phys. Chem. Chem. Phys., 24, 12116-12120 (2022).

(325) "Electronegativity: A Continuing Enigma"
P. Politzer and J. S. Murray, J. Phys. Org. Chem., e4406 (2022).

(326) "Thiazolium Salts as Chalcogen Bond Donors"
K. Konidaris, A. Daolio, A. Pizzi, P. Scilabra, G. Terraneo, S. Quici, J. S. Murray, P. Politzer and G. Resnati, Cryst. Growth Des., 22, 4987-4995 (2022); DOI: 10.1021/acs.cgd.2c00510.

(328) "Atoms Do Exist in Molecules: Analysis Using Electrostatic Potentials at Nuclei"
P. Politzer and J. S. Murray, Mol. Phys., e2101563 (2022), DOI: 10.1080/00268976.2022.2101563.

(329) "σ-Hole Interactions Involving a Group 7 Metal: Close Contacts in Neutral and Anionic Rhenium Derivatives"
A. Daolio, A. Pizzi, M. Calabrese, N. Demitri, J S. Murray, P. Politzer and G. Resnati, Cryst. Growth Des., 23, 574-579 (2023); DOI: 10.1021/acs.cgd.2c01180.

(330) "Intramolecular Repulsion Visible through the Electrostatic Potential in Disulfides: Analysis Via Varying Iso-density Envelopes"
G. Roos and J. S. Murray, J. Phys. Chem. A, 127, 8354-8364 (2023).

(331) "The Formation of σ-Hole Bonds: A Physical Interpretation"
J. S. Murray, Molecules, 29, 600(1-10) (2024).

(332) "Anisotropies in Electron Densities and Electrostatic Potentials of Halonium Ions: Focus on Chlorine, Bromine and Iodine"
P. Ramasami and J. S. Murray, J. Mol. Model., 30, 81(1-6) (2024), DOI: 10.1007/s00894-024- 05869-5.

(333) "Probing intramolecular interactions using molecular electrostatic potentials: Changing electron density contours to unveil both attractive and repulsive interactions"
G. Roos and J. S. Murray, Phys. Chem. Chem. Phys., 26, 7592-7601 (2024).

(334) "In memoriam: Peter Politzer: A life to be truly celebrated.
J. S. Murray, Struct. Chem., 35, 1335-1340 (2024); DOI: 10.1007/s11224-024-02339-9.

(335) "Radial behavior of electrostatic potentials of atoms and ions revisited: Isotropy and anisotropy"
P. Ramasami and J. S. Murray, ChemPhysChem, 25, e202400450 (2024).

(336) "Correspondence between the reaction force minimum and the onset of abrupt variations of the kinetic and potential energies in bond dissociation and formation"
P. Politzer, S. Gutiérrez-Oliva, T. Clark, J. S. Murray, J. Mol. Model., 30, 300 (2024); DOI: 10.1007/s00894-024-06101-0.

(337) "Atoms in molecules without boundaries: Analyses via electrostatic potentials at nuclei"
J. S. Murray, Struct. Chem., 35, 1355-1364 (2024); DOI: 10.1007/s11224-024-02369-3.

(338) "A revival of molecular surface electrostatic potential statistical quantities: Ionic solids and liquids"
J. S. Murray, K. E. Riley, T. Brinck, Crystals, 14, 995(1-11) (2024), DOI: 10.3390/cryst14110995.

(339) "No boundaries and naturally-defined boundaries obtained via the electrostatic potential"
G. Roos, D. E. P. Vanpoucke, J. S. Murray, ChemPhysChem, 26, e202401065(1-10) (2025), DOI: 10.1002/cphc.202401065.

(340) "Surface electrostatic potentials and average local ionization energies: Recent developments and applications"
J. S. Murray, chapter for Sokalski volume, 2025.

(341) "Electrostatic potentials of σ-holes and π-holes: A historical perspective"
J. S. Murray, in Theoretical and Computational Chemistry (S. J. Grabowski, ed), 2025, Ch. 4.

(342) "A theoretical journey delving into triel bonding: Anomalies, interpretations and applications"
T. Brinck, J. S. Murray, in Theoretical and Computational Chemistry (S. J. Grabowski, ed), 2025, Ch. 9, pp 219-137.

(343) "Electrostatic potentials at nuclei for atoms from Z=1 to Z=54 using the aHGBSP1-5 basis set"
M. Milovanović, J. S. Murray, J. Comput. Chem., 2025, DOI: 10.1002/jcc.70223.

(344) "Quantifying water hydrogen bonding from the surface electrostatic potential"
G. Roos, D. E. P. Vanpoucke, R. Blossey, M. F. Lensink and J. S. Murray, J. Chem. Phys., 163, 114112 (2025); DOI: 10.1063/5.0268712.

(345) "Short halogen-carbon bonds in 1-chloro- and 1-bromo-1-nitro-2,3-difluorocyclopropanes: Synergistic 1,4-intramolecular interactions?"
P. Ramasami, G. Roos, J. S. Murray, Struct. Chem., 2025, DOI: 10.1007/s11224-025-02639-8.

(346) "The anomalous nature of fluorine revisited: Amazing consequences"
J. S. Murray, *Phys. Chem. Chem. Phys.*, 2025, DOI: 10.039/D5CP03714J.

(347) "A computational renaissance in high-energy density materials (HEDMs) research"
H. Gao, J. S. Murray, J. M. Shreeve, Chem. Rev., 2025, in press.

VOLUMES EDITED:

Co-editor (with P. Politzer), *Quantitative Treatments of Solute/Solvent Interactions*, Elsevier, Amsterdam, 1994.

Co-editor (with K. D. Sen), *Molecular Electrostatic Potentials: Concepts and Applications*, Elsevier, Amsterdam, 1996.

Co-editor (with P. Politzer), *Energetic Materials: Part 1, Molecular and Crystal Properties*, Decomposition, Elsevier, Amsterdam, 2003.

Co-editor (with P. Politzer), *Energetic Materials: Part 2, Detonation, Combustion*, Elsevier, Amsterdam, 2003.