

I. Refereed Journal and Book Chapter Publications

- Sarah A. Ayoub and Jolanta B. Lagowski, "Optimizing the Performance of Multilayered Organic Polymer Devices Using Computational Dimer Approach A Case Study," *J. Phys. Chem. C*, 120, 496-507, 2016 (doi:10.1021/acs.jpcc.5b11150).
- Lin Ling and Jolanta B. Lagowski, "DFT Study of Electronic Band Structure of Alternating Triphenylamine-Fluorene Copolymers," *Polymer*, 54, 2535-2543, 2013 (doi:10.1016/j.polymer.2013.03.021).
- Mohammad J. Eslamibidgoli and Jolanta B. Lagowski, "The Effect of Side-Chain Length on the Solid-State Structure and Optoelectronic Properties of Fluorene-alt-Benzothiadiazole Based Conjugated Polymers-A DFT Study," *J. Phys. Chem. A*, 116, 10597-10606, 2012 (doi:10.1021/jp304974p).
- Yaping Li and Jolanta B. Lagowski, "A Multi-Step Simulation of Electron Mobility in Fluorene-Benzothiadiazole Conjugated Polymer - Case Study," *Comp. Theo. Chem.*, 977, 157-162 (2011) (doi:10.1016/j.comptc.2011.09.020).
- Yaping Li and Jolanta B. Lagowski, "Charge Carrier Mobility in Conjugated Organic Polymers - Case Studies Using Multi-Step Computational Approach," *Polymer*, 52, 4841-4850 (2011) (doi:10.1016/j.polymer.2011.08.011).
- Yaping Li and Jolanta B. Lagowski, "Charge Carrier Mobility in Conjugated Organic Polymers - Simulation of an Electron Mobility in a Carbazole-Benzothiadiazole Based Polymer," *Photonics North 2011* ed. R. Kashyap, M. Tetu, R. Kleiman, Proc. SPIE 8007, 80071Z (2011) (doi:10.1117/12.905452).
- Lin Ling and Jolanta B. Lagowski, "Electronic Band Structure of Alternating Fluorene-Oxadiazole Conjugated Copolymer - A 1D solid-state DFT study," *J. Mol. Struct. (Theochem)*, 944, 146-155 (2010) (doi:10.1016/j.theochem.2009.12.043).
- Yaping Li and Jolanta B. Lagowski, "Electric Field Effects on Bipolaron Transport in Heterocyclic Conjugated Polymers with Applications to Polythiophene," *Optical Materials*, 32, 1177-1187 (2010) (doi:10.1016/j.optmat.2010.03.028).
- Zhijun Gong and Jolanta B. Lagowski, 2009, "Theoretical Study of the Electronic and Optical Properties of Fluorene-Thieno[3,2-b]thiophene-Based Conjugated Copolymers," *Mol. Simul.*, 35, 737-747 (2009) (doi:10.1080/08927020902833079).
- Z. Gong and J.B. Lagowski, "Theoretical Study of the Structures and Electronic Properties of the Dimers of Fluorene and Carbazole and their Derivatives," *J. Mol. Struct. (Theochem)*, 866, 27-33 (2008) (doi: 10.1016/j.theochem.2008.06.034).
- S. Ferdous, and J.B. Lagowski, "A Comparison of Ground and Excited State Polarizabilities of Thiophene, Cyclopentadiene and Fulvene and their Cyano Substituted Oligomers - Ab Initio Study," *J. Pol. Sci. B: Polymer Physics*, 45, 1983-1995 (2007) (doi: 10.1002/polb.21190).
- Z. Gong and J.B. Lagowski, "Singlet Excitation Energies of Thiophene Derivatives of Fluorene: TD-DFT Study," *Int. J. Quant. Chem.*, 107, 159-171 (2007) (doi: 10.1002/qua.21030).
- D. Pavel, J.B. Lagowski and C.J. Lepage, "Computationally Designed Monomers for Molecular Imprinting of Chemical Warfare Agents - Part V," *Polymer*, 47, 8389-8399 (2006) (doi: 10.1016/j.polymer.2006.09.067).
- D. Pavel and J.B. Lagowski, "Computationally Designed Polymers for Molecular Imprinting of Theophylline and its Derivatives - Part IV," chapter "Advanced Research in Polymer Science" ed. F. Awaja, Research Signpost and Transworld Research Network (2006).
- D. Pavel and J.B. Lagowski, "Computationally Designed Copolymers for Molecular Imprinting of Theophylline and its Derivatives - Part III," chapter "Advanced Research in Polymer Science" ed. F. Awaja, Research Signpost and Transworld Research Network (2006).
- D. Pavel and J. B. Lagowski, "Computationally Designed Monomers and Polymers for Molecular Imprinting of Theophylline - Part II," *Polymer*, 46, 7543-7556 (2005) (doi: 10.1016/j.polymer.2005.05.146).
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- Z. Gong and J.B. Lagowski, "Electronic Structure Properties of Fluorene-Phenylene Monomer and its Derivatives: TD-DFT Study," *J. Mol. Struct. (Theochem)*, **729**, 211-222 (2005) (doi: 10.1016/j.theochem.2005.06.009).
- D. Chakraborty and J.B. Lagowski, "Geometry Relaxation in Singlet Excited States of Oligomers Containing Cyclopentadiene and Fulvene and their Cyano Derivatives," *Polymer*, **45**, 1331-1344 (2004) (doi: 10.1016/j.polymer.2003.04.004).
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- U. Salzner, J.B. Lagowski, P.G. Pickup and R.A. Poirier, "Theoretical Analysis of Effects of π -Conjugating Substituents on Building Blocks for Conducting Polymers," *J. Org. Chem.*, **64**, 7419-7425 (1999).
- A.V. Raja and J.B. Lagowski, "Modeling Thionylphosphazene Polymers With Short Model Compounds," *J. Mol. Struct. (Theochem)*, **465**, 93-109 (1999).
- U. Salzner, J.B. Lagowski, P.G. Pickup and R.A. Poirier, "An Accurate Method for Obtaining Band Gaps in Conducting Polymers Using a DFT/Hybrid Approach," *J. Phys. Chem.*, **102**, 2572-2578 (1998).
- U. Salzner, J.B. Lagowski, R.A. Poirier, and P.G. Pickup, "Comparison of Electronic Structures of Polycyclopentadiene, Polypyrrole, Polyfuran, Polysilole, Polyphosphole, Polythiophene, Polyselenophene, and Polytellurophene," *Synth. Met.*, **96**, 177-189 (1998).
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- J.B. Lagowski and J. McKenna, "Women Physics Faculty in Canada," *Physics in Canada*, **52**, 106 (1996).
- J.B. Lagowski, R. Jaeger, I. Manners and G.J. Vancso, "Ab Initio Study of the Structure in Poly(diphenoxythionylphosphazene)," *J. Mol. Struct. and Conf. (Theochem)*, **339**, 169-177 (1995).
- A.V. Raja and J.B. Lagowski, "Conformational Study of Halogen and Hydrogen Substituted Poly(thionylphosphazenes) Using Density Functional Theory Method," *Int. J. Quant. Chem.*, **54**, 117-136 (1995).
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- J.B. Lagowski and R. Jaeger, "An Ab Initio Study of the Structures of Poly(thionylphosphazenes) Mimics with H, Cl, CH₃ Side Groups: 3-21G* and 6-31G* Basis Sets Comparison," *Int. J. Quant. Chem.*, **53**, 321-334 (1995).
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II. Non-Refereed Contributions, Reports and Presentations at Conferences*

- **M. J. Eslamibidgoli** and J.B. Lagowski, “The Effect of Side-Chain Length on the Solid State Structure and Optical Properties of F8BT - A DFT Study ,” APS March Meeting, Boston, Massachusetts (Feb. 27-March 2, 2012).
- **H. Hussin** and J.B. Lagowski, “The Effect of a Solvent on the Structure, Energy, Dipole Moment and Transport Properties of Organic Conjugated Polymers,”; **Y. Li** and J.B. Lagowski, “Charge Carrier Mobility in Conjugated Organic Polymers - A Multi-Step Computational Approach,” CAP Congress, St. John’s (June 13-17, 2011).
- **Y. Li** and **J.B. Lagowski**, “Charge Carrier Mobility in Conjugated Organic Polymers - Case Studies Using Multi-Step Computational Approach,” Photonics North 2011, Ottawa (May 16-18, 2011).
- **Y. Li** and **J.B. Lagowski**, “Charge Carrier Mobility in Conjugated Organic Polymers - A Multi-Step Computational Approach,” APS March Meeting, Dallas, Texas (March 2011).
- **Y. Li** and J.B. Lagowski, “Charge Transport in Organic Conjugated Polymers Used in Solar Cells - A Computational Study,” APS March Meeting, Portland, Oregon (March 15-19, 2010).

- J.B. Lagowski, "Electronic and Charge Transport Properties of Conducting Polymers and Oligomers," Invited Talk, Theory Canada 5, Fredericton, NB (June 3-6, 2009).
- **Y. Li** and J.B. Lagowski, "Electric Field and Electron-Electron Interactions Effects on Bipolaron Transport in Polythiophene,"; **J.B. Lagowski** and Z. Gong, "Theoretical Studies of the Structures and Optical Properties of the Dimers of Fluorene and Carbazole Derivatives," APS March Meeting, New Orleans (March 2008).
- **Z. Gong** and J.B. Lagowski, "Theoretical Studies of the Electronic and Optical Properties of Fluorene-Based Conjugated Copolymers,"; **L. Ling** and J.B. Lagowski, "DFT Study of Band Structure on PA and OLED Materials,"; **Y. Li** and J.B. Lagowski, "Electric Field Effects on Bipolaron Transport in Polythiophene," 16th Canadian Symposium on Theoretical Chemistry, St. John's (August 4-9, 2007).
- **L. Ling** and J.B. Lagowski, "DFT Study of Band Structures of Organic Light-Emitting Materials," CAP Congress, Saskatoon (June 17-20, 2007).
- **J.B. Lagowski** and Z. Gong, "Electronic Structure Properties of Phenylene and Thiophene Derivatives of Fluorene: TD-DFT Study, 6th Canadian Computational Chemistry Conference, Vancouver (July 26-30, 2006).
- R. Barjovanu, F. Bensebaa, M. Day, J. Ding, **K. Faid**, A.A. Farah, C. Jackson Lepage, J. Lagowski, Z. Li, D. Kingston, S. Owega, D. Pavel, Ch. Py, K. Tufa, R. Voicu, "Development of 2D Molecular Imprinting Techniques, 3rd CRTI Summer Symposium, Quebec (June 20-24, 2005).
- **J.B. Lagowski** and S. Ferdous, "Ab Initio Study of Polarizabilities of Oligothiophene, Oligocyclopentadiene and Oligofulvene and their Cyano Substituted Oligomers," Bull. Am. Phys. Soc., **50**, APS March Meeting, Los Angeles (March 2005).
- D. Pavel and J.B. Lagowski, **final technical report** submitted to Y. Tao, IMS, NRC summarizing our computational contributions to the CRTI project entitled "Computationally Designed Molecularly Imprinted Monomers and Polymers," (March 2005).
- D. Pavel and J.B. Lagowski, **final (end of the year) technical report** submitted to K. Faid, IMS, NRC summarizing our computational contributions to the CRTI project entitled "Computationally Designed Molecularly Imprinted Monomers and Polymers," (January 2005).
- **J.B. Lagowski**, "Electronic Properties of Conducting Polymers and Oligomers," Memorial Symposium on Molecular Informatics, Modelling and Simulations, St. John's, Newfoundland (June 23, 2004).
- **K. Faid**, R. Voicu, A. Farah, C. Py, R. Barjovanu, F. Bensebaa, K. Tufa, Z. Li, J.B. Lagowski, D. Pavel, J.-F. Legault and C. Jackson Lepage, "Development of a Novel Molecular Imprinting Methodology for Sensing Applications," CRTI Summer Symposium, Gatineau, Quebec (June 15-16, 2004).
- **S. Ferdous** and J.B. Lagowski, "Ab Initio Polarizabilities of Conducting Polymers," CAP Congress, Winnipeg (June 13-16, 2004).
- **D. Pavel**, K. Faid and J.B. Lagowski, "Computationally Designed Monomers and Polymers for Molecular Imprinting," 87th Canadian Chemistry Conference, London, Ontario (May 29-June 1, 2004).
- D. Pavel and J.B. Lagowski, **15 monthly technical reports** submitted to K. Faid, IMS, NRC entitled "Computationally Designed Molecularly Imprinted Materials for Sensing Applications," 9 reports in 2003 and 11 reports in 2004.
- **K. Faid**, R. Voicu, A. Farah, C. Py, R. Barjovanu, F. Bensebaa, K. Tufa, Z. Li, J. Lagowski, D. Pavel, J.-F. Legault and C. Jackson Lepage, "Development of a Novel Molecular Imprinting Methodology for Sensing Applications," Proceedings of 2004 CRTI Summer Symposium, Gatineau, Quebec (June 2004).
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- **Z. Gong** and J.B. Lagowski, "Excitation Energies of Fluorene-Based Polymers and Oligomers - Ab Initio Approach," Bull. Am. Phys. Soc., **48**, APS March Meeting, Austin (March 2003).
- **J.B. Lagowski**, "Ab Initio Study of Excitation Energies of End-Substituted Phenylene Vinylene Oligomers," CAP Congress, Quebec (June 2002).

- **J.B. Lagowski**, “Ab Initio Investigation of Conformational and Excitation Energies of Phenylene Vinylene Oligomers,” Workshop on Photonics and Electronics of Organic Materials IMS, NRC and Canadian Symposium on Theoretical Chemistry, Ottawa (August 2001).
- **D. Chakraborty** and **J.B. Lagowski**, “Ab Initio Investigation of Excitation Energies of Thiophene, Cyclopentadiene and Fulvene based π -Conjugated Polymers,” CAP Congress, Toronto (June 2000).
- **D. Chakraborty**, **H. Subramanian** and **J.B. Lagowski**, “Excited State Study of Thiophene, Cyclopentadiene and Fulvene Based Polymers,” Bull. Am. Phys. Soc., **44**, APS March Meeting, Atlanta (1999).
- **J.B. Lagowski** and **H. Subramanian**, “Trends in Electronic Properties of Thiophene, Cyclopentadiene and Fulvene Based Polymers: Comparison of Ab Initio and Semi-empirical Calculations,” Bull. Am. Phys. Soc., **43**, APS March Meeting, Los Angeles, (March 1998).
- **J.B. Lagowski**, “Computer Simulations of Polymers – Quantum Mechanical Studies,” Computational Physics Symposium, CAP Congress, Calgary, Alberta (invited talk) (June 1997).
- **U. Salzner**, **J.B. Lagowski**, **P.G. Pickup** and **R.A. Poirier**, “Design of Conducting Polymers Employing Density Functional Theory,” Bull. Am. Phys. Soc., **42**, APS March Meeting, Kansas City, Missouri (March 1997).
- **W. Li** and **J.B. Lagowski**, “Ab Initio Study of the Structure of Phospholipid Head Groups,” 28th Canadian High Polymer Forum, Sarnia, Ontario, (August 1996).
- **U. Salzner**, **J.B. Lagowski**, **P.G. Pickup** and **R.A. Poirier**, “Design of Low Band Gap Organic Polymers Employing Ab Initio Calculations and Electronic Structure Analysis,” 79th CSC Conference, St. John’s, Newfoundland (June 1996).
- **H. Subramanian** and **J.B. Lagowski**, “Investigation of Electronic Properties of Conducting Polymers Using Semi-Empirical Approach,” 79th CSC Conference, St. John’s, Newfoundland (June 1996)
- **H. Subramanian** and **J.B. Lagowski**, “Investigation of Electronic Properties of Conducting Polymers Using Semi-Empirical Approach,” 1996 Electronic Structure Workshop, Eighth Annual Conference on New Methods in Electronic Structure Calculations, Minneapolis, Minnesota, USA (June 1996).
- **A.V. Raja** and **J.B. Lagowski**, “Bonding in Thionylphosphazene Systems: Comparison of the Electronic Structures of Long, Short and Cyclic Mimics of Compounds of Type S(OX)(R₂PN)₂,” 79th CSC Conference, St. John’s, Newfoundland (June 1996).
- **H. Subramanian** and **J.B. Lagowski**, “Investigation of Electronic Structure in Organic Polymers Possessing Very Low Intrinsic Bandgaps,” Canadian Symposium on Theoretical Chemistry, Fredericton, New Brunswick (August 1995).
- **J.B. Lagowski** and **A.V. Raja**, “Correlating Single Chain Flexibility with Glass Transition Temperatures in Polyphosphazenes,” CAP Congress, Quebec, Quebec (June 1995).
- **W. Li** and **J.B. Lagowski**, “Ab Initio Study of the Structure of the Phospholipid Headgroups,” CAP Congress, Quebec, Quebec (June 1995).
- **A.V. Raja** and **J.B. Lagowski**, “Investigation of Structure and Bonding in Phosphorus Based Inorganic Polymers Using Density Functional Method,” CAP Congress, Quebec, Quebec (June 1995).
- **A.V. Raja** and **J.B. Lagowski**, “Conformational Study of Substituted Poly(thionylphosphazenes) Molecular Models Using Density Functional Theory,” Second Canadian Computational Chemistry Conference, Kingston, Ontario (May 1994).
- **A.V. Raja** and **J.B. Lagowski**, “Substituted Poly(thionylphosphazenes) Molecular Models – Study of Cis–Trans Conformations Using Density Functional Theory Approach,” Bull. Am. Phys. Soc., **39**, APS March Meeting, Division of High Polymer Physics, Pittsburgh, Pennsylvania (March 1994).
- **A.V. Raja** and **J.B. Lagowski**, “Substituted Poly(thionylphosphazenes) Molecular Models – Study of “Twisted” Cis–Trans Conformations Using Density Functional Theory Approach,” Poster, ACS, Division of Polymer Chemistry, “Molecular Simulations of Structure and Properties in Polymer Systems,” Pacific Grove, California (October 1993).

- **G.J. Vancso**, J.B. Lagowski, R. Jaeger and I. Manners, "Structure and Dynamics of Organic and Inorganic Macromolecules Studied via Computer Modeling of Mimics," Twenty-Seventh Canadian High Polymer Forum, Gananoque, Ontario (August 1993).
- J.B. Lagowski, **R. Jaeger**, I. Manners and G.J. Vancso, "Ab Initio Studies on Mimics of Substituted Poly(thionylphosphazenes)," ACS, Division of Polymer Chemistry, Denver, Colorado (March/April 1993).
- **J.B. Lagowski** and G. J. Vancso, "Modeling Conformational States of Polystyrene by an Ab Initio Study of Diphenylpentane," APS, Division of Polymer Physics, (March 1993).
- **J.B. Lagowski** and G.J. Vancso, "Short Range Molecular Order In Relaxed And Oriented Glassy Polystyrene: A Comparative Study Using X-Ray Scattering and Molecular Modeling Techniques," Canadian Society of Chemists Conference, Hamilton, (June 1991).
- **J.B. Lagowski** and G.J. Vancso, "Ab Initio Study of the Conformations of Isopropylbenzene and Phenylbutane," First Canadian Symposium on Computational Chemistry, Orford, Quebec (May 1991).
- **J.B. Lagowski** and J. Noolandi, "New Theory of Semiflexible Liquid Crystal Polymers," The 13th International Liquid Crystal Conference, Vancouver, B.C. (July 1990).
- **S.H. Vosko** and J.B. Lagowski, "Negative Ions in the Fourth Period: Some Surprises in their Electron Configurations," 3rd Chemical Congress of North America, Toronto, Ontario (June 1988) (invited talk, Division of Physical Chemistry).
- **J.B. Lagowski** and S.H. Vosko, "Density Functional Theory of the Odd Parity Bound States in the 3d Series Negative Ions," Bull. Am. Phys. Soc., **33**, APS March Meeting, New Orleans (March 1988).
- **J.B. Lagowski** and S.H. Vosko, "The Ground States of Ca^- and Sc^- from the Density Functional Point of View," CAP Congress, Toronto (May 1987).
- **J.B. Lagowski** and S.H. Vosko, "A Comparison of Various Local and Nonlocal Correlation Energy Functionals," Bull. Am. Phys. Soc., **32**, APS March Meeting, New York (March 1987).

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