I. Refereed Journal and Book Chapter Publications

- Sarah A. Ayoub and Jolanta B. Lagowski, "Optimizing the Performance of the Bulk Heterojunction Organic Solar Cells - Some General Guidelines Obtained from the DFT Investigation," Materials and Design, 2017 (under review).
- M.Z.H. Khan, S. Aljohani, A. Alrawashdeh, Y. Zhao and J.B. Lagowski, "DFT Investigation of the Interaction between the Single-walled Carbon Nanotubes and Fluorene-based Conjugated Oligomers," Chem. Phys. Phys. Chem., 19, 28071-28082, 2017 (doi: 10.1039/c7cp04851c).
- S. Aljohani, M.Z.H. Khan, A. Alrawashdeh, Y. Zhao and J.B. Lagowski, "Interactions between Single-walled Carbon Nanotubes and Oligophenylene Ethynylenes: A DFT Study," J. Phys. Chem. C, 121, 4695-4702, 2017 (doi:10.1021/acs.jpcc.6b12747).
- Sarah A. Ayoub and Jolanta B. Lagowski, "Optimizing the Performance of Multilayered Organic Polymer Devices Using Computational Dimer ApproachA Case Study," J. Phys. Chem. C, 120, 496-507, 2016 (doi:10.1021/acs.jpcc.5b11150).
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II. Non-Refereed Contributions, Reports and Presentations at Conferences*

- **S. Ayoub** and J.B. Lagowski, "A DFT Investigation of Conjugated Polymers/Oligomers and Fullerenes Interactions in Bulk Heterojunction Organic Solar Cells," Oral Presentation, International Conference on Advances in Functional Materials, Los Angeles, USA, Aug. 14-17, 2017
- S. Ayoub and **J.B. Lagowski**, "A DFT Investigation of Conjugated Polymers/Oligomers and Fullerenes Interactions in Bulk Heterojunction Organic Solar Cells, " Poster, CAP Congress, Kingston, Ontario (May 28 -June 2 2017).

- **J.B. Lagowski**, "Investigations of the Intermolecular Interactions between Organic Conjugated Monomers, and Conjugated Oligomers and Nanotubes Using Dispersion-Corrected DFT," **Invited Talk**, CAP Congress, Ottawa, Ontario (June 13-17, 2016).
- S. Ayoub and **J.B. Lagowski**, "Investigation of Intermolecular Interactions between Fluorene-based Conjugated Polymers Using the Dispersion-corrected DFT," APS March Meeting, San Antonio, Texas, March 2-6, 2015, and International Conference on Advances in Functional Materials -2015, Stony Brook, New York, June 29 July 3, 2015 (awarded first place in the poster session).
- **M.Z. H. Khan** and J.B. Lagowski, "Investigation of the Interaction between the Single Walled Carbon Nanotube and Fluorene-based Conjugated Oligomers Using Various Dispersion Correction DFT Methods," CAP Congress, Edmonton, Alberta , June 15-19, 2015.
- **J.B. Lagowski**, "Modeling the Structure, Optoelectronic Properties and Charge Transport of Organic Semiconducting Cpnjugated Polymers with DFT," **Invited Talk**, CAP Congress, Sudbury, Ontario (June 16-20, 2014).
- 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 ," Materials Research Society, Boston, Massachusetts (Dec. 1-6, 2013).
- **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).
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- **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 $S(OX)(R_2PN)_2$," 79^{th} CSC Conference, St, John's, Newfoundland (June 1996).
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- **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).
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- **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).

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*Bold–faced names indicate the presenter.