Curriculum Vitae

Dr. Erin R. Johnson

Department of Chemistry, Dalhousie University
6274 Coburg Road, Halifax, NS, Canada, B3H 4R2
E-mail: erin.johnson@dal.ca
Website: http://schooner.chem.dal.ca

Academic Appointments

3. Jul. 2018 – onwards. Full Professor of Chemistry at Dalhousie University (Halifax, Canada); Herzberg-Becke Chair in Theoretical Chemistry. Cross-appointed to the Department of Physics and Atmospheric Science.

2. Jul. 2015 – Jun. 2018. Associate Professor of Chemistry at Dalhousie University (Halifax, Canada); Herzberg-Becke Chair in Theoretical Chemistry. Cross-appointed to the Department of Physics and Atmospheric Science.

1. Jul. 2010 – Jun. 2015. Assistant Professor of Chemistry at the University of California, Merced. Awarded tenure and promotion to Associate Professor, to be effective July 2015.

Professional Preparation

4. Jan. 2008 – Jun. 2010. NSERC Postdoctoral Fellowship held in the Department of Chemistry at Duke University (Durham, USA), under the supervision of Prof. Weitao Yang.

3. Sep. 2004 – Dec. 2007. Ph.D. in Chemistry from Queen's University (Kingston, Canada). Thesis work was completed under the supervision of Prof. Axel D. Becke, entitled "A Density-Functional Theory Including Dispersion Interactions."

2. May – Aug. 2004. Summer research fellow at the National Institute for Nanotechnology, National Research Council of Canada (Edmonton, Canada), under the supervision of Dr. Gino A. DiLabio.

1. Sep. 2000 – Apr. 2004. B.Sc. with Honours in Integrated Science (chemistry/mathematics) from Carleton University (Ottawa, Canada).

Research Interests

Development and applications of density-functional theory for study of electronic structure. Current applications include London dispersion interactions, molecular crystals, layered materials, electrides, and organometallic complexes.

Supervision of Highly-Qualified Personnel

To date, I have been an advisor to 3 post-doctoral fellows, 7 Doctoral students, 5 Master's students, and 9 undergraduates conducting research in my group.

Awards and Honours

8. 2020. Rutherford Memorial Medal in Chemistry; awarded by the Royal Society of Canada for outstanding research in any branch of chemistry, with preference given to candidates under the age of forty.

7. 2019. E.W.R. Steacie Memorial Fellowship; awarded by NSERC to enhance the career development of outstanding and highly promising scientists and engineers who are faculty members of Canadian universities.

6. 2018. Dirac Medal; awarded by the World Association of Theoretical and Computational Chemists to an outstanding theoretical and computational chemist under the age of forty.

5. 2018. Tom Ziegler Award; awarded by the Canadian Society for Chemistry to a scientist who has made an outstanding early-career contribution to theoretical and/or computational chemistry.

4. 2018. Faculty of Science Killam Prize; awarded by Dalhousie University in recognition of exceptional research accomplishments by faculty who have obtained their doctorate within the preceding eleven years.

3. 2016. CMOA Promising Scientist Award; awarded by the Centre de Mécanique Ondulatoire Appliquée/Center for Applied Wave Mechanics to leading researchers in Quantum Chemistry and Physics under the age of thirty-five.

2. 2006. André Hamer Postgraduate Prize; awarded to the top-ranked student in the NSERC Ph.D. fellowship competition.

1. 2004. Governor General's academic medal; awarded for the highest undergraduate graduating average (4.0 GPA) at Carleton University.

Published Papers

123 peer-reviewed articles, 16150 total citations, h-index of 41, i10-index of 90 (Google Scholar). Only papers published within the last 5 years are shown.

50. M. A. White, S. Kahwaji, V. F. S. Freitas, R. Siewert, J. A. Weatherby, M. D. M. C. Ribeiro da Silva, S. P. Verevkin, E. R. Johnson, and J. W. Zwanziger, Relative Thermodynamic Stability of Diamond and Graphite. Angew. Chem. Int. Ed. 2020, DOI: 10.1002/anie.202009897

49. A. Otero de la Roza and E. R. Johnson, Application of XDM to Ionic Solids: the Importance of Dispersion for Bulk Moduli and Crystal Geometries. J. Chem. Phys. **153**, 054121, 2020.

48. A. N. Sharma, L. Grandinetti, E. R. Johnson, M. St. Maurice, and S. L. Bearne, Potent Inhibition of Mandelate Racemase by Boronic Acids: Boron as a Mimic of a Carbon Acid Center. Biochem. **59**, 3026-3037, 2020.

47. J. W. M. MacMillan, K. M. Marczenko, E. R. Johnson, and S. S. Chitnis, Hydrostibination of alkynes: A radical mechanism. Chem. Eur. J. 2020, DOI: 10.1002/chem.202003153

46. A. J. Price and E. R. Johnson, Theoretical Investigation of Amino-Acid Adsorption on Hydroxylated Quartz Surfaces: Dispersion can Determine Enantioselectivity. Phys. Chem. Chem. Phys. **22**, 16571-16578, 2020. PCCP HOT article.

45. X. Feng, A. D. Becke, and E. R. Johnson, Computational Modeling of Piezochromism in Molecular Crystals. J. Chem. Phys. **152**, 234106 (2020).

44. A. Otero de la Roza, L. M. LeBlanc, and E. R. Johnson, What is "Many-Body" Dispersion and Should I Worry About it? Phys. Chem. Chem. Phys. Invited perspective. **22** 8266-8276 (2020). PCCP HOT article.

43. A. Otero de la Roza, L. M. LeBlanc, and E. R. Johnson, Asymptotic Pairwise Dispersion Corrections Can Describe Layered Materials Accurately. J. Phys. Chem. Lett. **11**, 2298-2302 (2020).

42. A. Otero-de-la-Roza and E. R. Johnson. Analysis of Density-Functional Errors for Non-Covalent Interactions Between Charged Molecules. J. Phys. Chem. A. Invited article. **124**, 353-361 (2020).

41. E. Awoonor-Williams, W. Isley III, S. G. Dale, B. Roux, A. D. Becke, H. Yu, E. R. Johnson, and C. N. Rowley. Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. J. Comp. Chem. Invited article. **41**, 427-438 (2020).

40. L. M. LeBlanc and E. R. Johnson. Crystal-Energy Landscapes of Active Pharmaceutical Ingredients Using Composite Approaches. CrystEngComm. **21**, 5995-6009 (2019).

39. A. Otero-de-la-Roza, L. M. LeBlanc, and E. R. Johnson. Dispersion XDM with Hybrid Functionals: Delocalization Error and Halogen Bonding in Molecular Crystals. J. Chem. Theory Comput. **15**, 4933-4944 (2019).

38. J. A. Noël, L. Kreplak, L. M. LeBlanc, D. S. Patterson, M. Fleischauer, E. R. Johnson, and M. A. White. Structure of Clusters in Liquid Fatty Acids and their Role in Nucleation. J. Phys. Chem. B. **123**, 7043-7054 (2019).

37. M. R. Vazirisereshk, H. Ye, A. Otero-de-la-Roza, Z. Ye, M. Zhao, A. T. C. Johnson, E. R. Johnson, R. W. Carpick, and A. Martini. Origin of Nanoscale Friction Contrast between Supported Graphene, MoS_2, and a Graphene/MoS_2 Heterostructure. Nano Lett. **19**, 5496-5505 (2019).

36. D. Santamaría-Pérez, D. Daisenberger, J. Ruiz-Fuertes, T. Marqueño, R. Chulia-Jordan, C. Muehle, M. Jansen, P. Rodriguez-Hernandez, A. Munoz, E. R. Johnson, A. Otero-de-la-Roza. Gold(I) Sulphide: Unusual Bonding and an Unexpected Computational Challenge in a Simple Solid. Chem. Sci. **10**, 6467-6475 (2019).

35. X. Feng, A. D. Becke, and E. R. Johnson. Becke's Virial Exciton Model Gives Accurate Charge-Transfer Excitation Energies. J. Chem. Phys. **149**, 231101 (2018).

34. S. G. Dale and E. R. Johnson. Theoretical Descriptors of Electrides. J. Phys. Chem. A. Invited feature article. **122**, 9371-9391 (2018).

33. L. M. LeBlanc, J. A. Weatherby, A. Otero-de-la-Roza, and E. R. Johnson. Non-Covalent Interactions in Molecular Crystals with Local Orbitals Using the Exchange-Hole Dipole Moment Model. J. Chem. Theory Comput. **14**, 5715-5724 (2018).

32. C. M. Lavoie, J. P. Tassone, M. J. Ferguson, Y. Zhou, E. R. Johnson, and M. Stradiotto. Probing the Influence of PAd-DalPhos Ancillary Ligand Structure on Nickel-Catalyzed Ammonia Cross-Coupling. Organometallics. **37**, 4015-4023 (2018).

31. S. G. Dale, A. D. Becke, and E. R. Johnson. Density-Functional Description of Alkalides: Introducing the Alkalide State. Phys. Chem. Chem. Phys. **20**, 26710-26718 (2018).

30. L. M. LeBlanc, S. G. Dale, C. R. Taylor, A. D. Becke, G. M. Day, and E. R. Johnson. Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acid-Base Co-Crystals. Angew. Chem. Int. Ed. VIP paper. **57**, 14906-14910 (2018).

29. A. Otero-de-la-Roza, A. Martín-Pendás, and E. R. Johnson. Quantitative electron delocalization in solids from maximally localized Wannier functions. J. Chem. Theory Comput. **14**, 4699-4710 (2018).

28. E. T. Walters, M. Mohebifar, E. R. Johnson, and C. N. Rowley. Evaluating the London Dispersion Coefficients of Protein Force Fields Using the Exchange-Hole Dipole Moment Model. J. Phys. Chem. B. **122**, 6690-6701 (2018).

27. A. D. Becke, S. G. Dale, and E. R. Johnson. Charge transfer in CT complexes from the Becke'05 density functional. J. Chem. Phys. **148**, 211101 (2018).

26. S. G. Dale, A. Otero-de-la-Roza, and E. R. Johnson. Pressure-Induced Isostructural Antiferromagnetic-Ferromagnetic Transition in an Organic Electride. J. Phys. Chem. C. **122**, 12742-12747 (2018).

25. T. Gould, E. R. Johnson, and S. A. Tawfik. Are dispersion corrections accurate outside equilibrium? A case study on benzene. Beilstein J. Org. Chem. **14**, 1181-1191 (2018). Invited article.

24. A. V. Gatien, C. M. Lavoie, R. N. Bennett, M. J. Ferguson, R. McDonald, E. R. Johnson, A. W. H. Speed, and M. Stradiotto. Application of Diazaphospholidine/Diazaphospholene-Based Bisphosphines in Room Temperature Nickel-Catalyzed C(sp2)-N Cross-Couplings of Primary Alkylamines with (Hetero)aryl Chlorides and Bromides. ACS Catalysis. **8**, 5328-5339 (2018).

23. M. S. Christian and E. R. Johnson. Effect of the Metal Substrate on Interlayer Interactions in Bilayer Graphene. J. Phys. Chem. C. **122**, 8910-8918 (2018).

22. L. M. LeBlanc, A. Otero-de-la-Roza, and E. R. Johnson. Composite and Low-Cost Approaches for Molecular Crystal Structure Prediction. J. Chem. Theory Comput. **14**, 2265-2276 (2018).

21. D. Chevrier, V. D. Thanthirige, Z. Luo, S. Driscoll, P. Cho, M. MacDonald, R. Guda, J. Xie, E. R. Johnson, A. Chatt, N. Zheng, and P. Zhang, The Structure of Highly Luminescent Protein-Stabilized Gold Nanoclusters. Chem. Sci. **9**, 2782-2790 (2018).

20. X. Feng, A. Otero-de-la-Roza, and E. R. Johnson. The Effect of Electronic Excitation on London Dispersion. Can. J. Chem. **96**, 730-737 (2018). Invited article.

19. B. Rice, L. M. LeBlanc, A. Otero-de-la-Roza, M. Fuchter, E. R. Johnson, J. Nelson, and K. Jelfs. A Computational Exploration of the Crystal Energy and Charge Carrier Mobility Landscapes of the Chiral [6]Helicene Molecule. Nanoscale. **10**, 1865-1876 (2018).

18. M. Mohebifar, E. R. Johnson, and C. N. Rowley, Evaluating Force-Field London Dispersion Coefficients Using the Exchange-Hole Dipole Moment Model. J. Chem. Theory Comput. **13**, 6146-6157 (2017).

17. S. R. Whittleton, A. Otero-de-la-Roza, and E. R. Johnson, Exchange-Hole Dipole Dispersion Model for Accurate Energy Ranking in Molecular Crystal Structure Prediction II: Non-Planar Molecules. J. Chem. Theory. Comput. **13**, 5332-5342 (2017).

16. C.-H. Tien, M. R. Adams, M. J. Ferguson, E. R. Johnson, and A. W. H. Speed, Synthesis and Catalytic Activity of 1,2,4,3-Triazaphospholenes. Org. Lett. **19**, 5565-5568 (2017).

15. S. G. Dale and E. R. Johnson, The Ionic Versus Metallic Nature of 2D Electrides: A Density-Functional Description. Phys. Chem. Chem. Phys. **19**, 27343-27352 (2017).

14. S. G. Dale, E. R. Johnson, and A. D. Becke, Interrogating the B05 Density Functional for Non-Locality Information. J. Chem. Phys. **147**, 154103 (2017).

13. M. S. Christian, A. Otero-de-la-Roza, and E. R. Johnson, Adsorption of Graphene to Metal (111) Surfaces using the Exchange-Hole Dipole Moment Model. Carbon. **124**, 531-540 (2017).

12. C. M. Lavoie, R. McDonald, E. R. Johnson, and M. Stradiotto, Bisphosphine-Ligated Nickel Pre-catalysts in C(sp^2)-N Cross-Couplings of Aryl Chlorides: A Comparison of Ni(I) and Ni(II). Adv. Synth. Catal. **359**, 2972-2980 (2017).

11. Y. Yang, B. Rice, X. Shi, J. R. Brandt, R. Correa da Costa, G. Hedley, D.-M. Smilgies, J. M. Frost, I. D. W. Samuel, A. Otero-de-la-Roza, E. R. Johnson, K. E. Jelfs, J. Nelson, A. J. Campbell and M. J. Fuchter, Emergent Properties of an Organic Semiconductor Driven by its Molecular Chirality. ACS Nano. **11**, 8329-8338 (2017).

10. E. R. Johnson and A. D. Becke, DFT Treatment of Strong Correlation in 3d Transition-Metal Diatomics. J. Chem. Phys. **146**, 211105 (2017).

9. S. G. Dale and E. R. Johnson, Thermodynamic Cycles of the Alkali Metal-Ligand Complexes Central to Electride Formation. Phys. Chem. Chem. Phys. **19**, 12816-12825 (2017).

8. M. S. Christian, A. Otero-de-la-Roza, and E. R. Johnson, Adsorption of Graphene to Nickel (111) using the Exchange-Hole Dipole Moment Model. Carbon. **118**, 184-191 (2017).

7. S. R. Whittleton, A. Otero-de-la-Roza, and E. R. Johnson, The Exchange-Hole Dipole Dispersion Model for Accurate Energy Ranking in Molecular Crystal Structure Prediction. J. Chem. Theory Comput. **13**, 441-450 (2017).

6. L. M. LeBlanc, A. Otero-de-la-Roza, and E. R. Johnson, Evaluation of Shear-Slip Transitions in Crystalline Aspirin by Density-Functional Theory. Cryst. Growth Des. **16**, 6867-6873 (2016).

5. S. G. Dale and E. R. Johnson, The Explicit Examination of the Magnetic States of Electrides. Phys. Chem. Chem. Phys. **18**, 27326-27335 (2016).

4. A. Otero-de-la-Roza, J. E. Hein, and E. R. Johnson, Reevaluating the Stability and Prevalence of Conglomerates: Implications for Preferential Crystallization. Cryst. Growth Des. **16**, 6055-6059 (2016).

3. M. S. Christian, A. Otero-de-la-Roza, and E. R. Johnson. Surface Adsorption from the Exchange-Hole Dipole Moment Dispersion Model. J. Chem. Theory Comput. **12**, 3305-3315 (2016).

2. A. Otero-de-la-Roza, G. A. DiLabio, and E. R. Johnson, Exchange-Correlation Effects for Non-Covalent Interactions in Density-Functional Theory. J. Chem. Theory. Comput. **12**, 3160-3175 (2016).

1. J. B. Dizon and E. R. Johnson. Van der Waals Potential Energy Surfaces from the Exchange-Hole Dipole Moment Dispersion Model. Can. J. Chem. Invited article. **94**, 1049-1056 (2016).

Book Chapters

2. E. R. Johnson, The Exchange-Hole Dipole Moment Dispersion Model. In: Non-Covalent Interactions in Quantum Chemistry and Physics, A. Otero de la Roza and G. DiLabio eds. (Elsevier, 2017) Ch. **5**, pp. 169-194.

1. A. Savin and E. R. Johnson. Judging Density-Functional Approximations: Some Pitfalls of Statistics. In: Density Functionals: Thermochemisty, Top. Curr. Chem. **365**, 81-95 (2015).