

Curriculum Vitae

Erin R. Johnson

Department of Chemistry, Duke University
Durham, NC, 27708
Phone: (919) 660-1640
Email: Erin.Johnson@duke.edu

Academics

2008-? Postdoctoral research in the Department of Chemistry at Duke University, under the supervision of Prof. Weitao Yang. Awarded NSERC Postdoctoral Fellowship.

2004-2007. Ph.D. in Chemistry from Queen's University. Awarded NSERC Canada Graduate Scholarships and the André Hamer Postgraduate Prize. Thesis work completed under the supervision of Prof. Axel D. Becke, entitled "A Density Functional Theory Including Dispersion Interactions."

2000-2004. B.Sc. with Honours in Integrated Science (chemistry/mathematics) from Carleton University. Awarded the Governor General's academic medal. Thesis work completed under the supervision of Dr. Gino A. DiLabio, entitled "Exploring Protein Folding using a Sequential Build-up Approach."

Published papers

1. A. D. Becke and E. R. Johnson, Exchange-Hole Dipole Moment and the Dispersion Interaction Revisited. *J. Chem. Phys.* **127**, 154108 (2007).
2. A. D. Becke and E. R. Johnson, A Unified Density-Functional Treatment of Dynamical, Nondynamical and Dispersion Correlations. *J. Chem. Phys.* **127**, 124108 (2007).
3. E. R. Johnson, R. M. Dickson, and A. D. Becke, Density Functionals and Transition-Metal Atoms. *J. Chem. Phys.* **126**, 184104 (2007).
4. G. A. DiLabio and E. R. Johnson, Lone Pair- π and π - π Interactions play an Important Role in Proton Coupled Electron Transfer Reactions. *J. Am. Chem. Soc.* **129**, 6199 (2007).
5. E. R. Johnson, D. J. J. McKay, and G. A. DiLabio, Hydrogen-Bond Strengths in Large Complexes: Efficient Calculations using Locally Dense Basis Sets. *Chem. Phys. Lett.* **435**, 201 (2007).

6. E. R. Johnson and A. D. Becke, Van der Waals Interactions from the Exchange Hole Dipole Moment: Application to Bio-Organic Benchmark Systems. *Chem. Phys. Lett.* **432**, 600 (2006).
7. A. D. Becke and E. R. Johnson, A Simple Effective Potential for Exchange. *J. Chem. Phys.* **124**, 221101 (2006).
8. E. R. Johnson and A. D. Becke, A Post-Hartree-Fock Model of Intermolecular Interactions: Inclusion of Higher-Order Corrections. *J. Chem. Phys.* **124**, 174104 (2006).
9. A. D. Becke and E. R. Johnson, Exchange-hole Dipole Moment and the Dispersion Interaction: High-Order Dispersion Coefficients. *J. Chem. Phys.* **124**, 014104 (2006).
10. E. R. Johnson and G. A. DiLabio, Structure and Binding Energies in van der Waals Dimers: Comparison between Density Functional Theory and Correlated Ab Initio Methods. *Chem. Phys. Lett.* **419**, 333 (2006).
11. A. D. Becke and E. R. Johnson, A Density-Functional Model of the Dispersion Interaction. *J. Chem. Phys.* **123**, 154101 (2005).
12. E. R. Johnson and A. D. Becke, A Post-Hartree-Fock Model of Intermolecular Interactions. *J. Chem. Phys.* **123**, 024101 (2005).
13. A. D. Becke and E. R. Johnson, Exchange-Hole Dipole Moment and the Dispersion Interaction. *J. Chem. Phys.* **122**, 154104 (2005).
14. G. A. DiLabio, R. A. Wolkow, and E. R. Johnson, Efficient Silicon Surface and Cluster Modeling Using Quantum Capping Potentials. *J. Chem. Phys.* **122**, 044708 (2005).
15. E. R. Johnson, R. A. Wolkow, and G. A. DiLabio, Reply to Comment on "Application of 25 Density Functionals to Dispersion-Bound Homomolecular Dimers." *Chem. Phys. Lett.* **401**, 595 (2005).
16. E. R. Johnson and G. A. DiLabio, A Theoretical Study of the Dispersion-Bound Silane-Methane Dimer. *Chem. Phys. Lett.* **397**, 314 (2004).
17. E. R. Johnson, R. A. Wolkow, and G. A. DiLabio, Application of 25 Density Functionals to Dispersion-Bound Homomolecular Dimers. *Chem. Phys. Lett.* **394**, 334 (2004).
18. E. R. Johnson, O. J. Clarkin, and G. A. DiLabio, Density Functional Theory based Model Calculations for Accurate Bond Dissociation Enthalpies. 3. A Single Approach for X-H, X-X, and X-Y (X, Y = C, N, O, S, Halogen) Bonds. *J. Phys. Chem. A* **107**, 9953 (2003).
19. P. Kruse, E. R. Johnson, G. A. DiLabio, and R. A. Wolkow, Patterning of Vinylferrocene on H-Si(100) via Self-Directed Growth of Molecular Lines and STM-Induced Decomposition. *Nano Lett.* **2**, 807 (2002).

20. M. C. Foti, E. R. Johnson, M. R. Vinqvist, J. S. Wright, L. R. C. Barclay, and K. U. Ingold, Naphthalene Diols: A New Class of Antioxidants. Intramolecular Hydrogen Bonding in Catechols, Naphthalene Diols, and Their Aryloxyl Radicals. *J. Org. Chem.* **67**, 5190 (2002).
21. J. S. Wright, E. R. Johnson, and G. A. DiLabio, Predicting the Activity of Phenolic Antioxidants: Theoretical Method, Analysis of Substituent Effects, and Applications to Major Families of Antioxidants. *J. Am. Chem. Soc.* **123**, 1173 (2001).

Conference talks

1. E. R. Johnson and A. D. Becke, A Unified Density-Functional Treatment of Dynamical, Nondynamical and Dispersion Correlations. Presented at the 90th Canadian Chemistry Conference, Winnipeg (2007).
2. E. R. Johnson and A. D. Becke, A Simple Effective Potential for Exchange. Presented at the Atlantic Theoretical Chemistry Symposium, St. Francis Xavier University (2006).
3. E. R. Johnson and A. D. Becke, Van der Waals Interactions from the Exchange Hole Dipole Moment. Presented at the 89th Canadian Chemistry Conference, Halifax (2006).
4. E. R. Johnson and A. D. Becke, Efficient Models of Dispersion from the Exchange Hole Dipole Moment. Presented at the Symposium on Chemical Physics, University of Waterloo (2005).
5. E. R. Johnson, A. D. Becke, and G. A. DiLabio, Applicability of Density Functional Theory for Structures and Binding Energies of van der Waals Complexes. Invited seminar presented to the Department of Chemistry at the University of Alberta (2005).
6. E. R. Johnson and A. D. Becke, A Post-Hartree-Fock Model of Intermolecular Interactions. Presented at the 88th Canadian Chemistry Conference, Saskatoon (2005).
7. E. R. Johnson and G. A. DiLabio, Effective Computational Modeling of Large Chemical Systems Using Quantum Capping Potentials. Presented at the Physical Organic Mini-Symposium, Queen's University (2004).

Conference posters

1. E. R. Johnson and A. D. Becke, A Unified Density-Functional Treatment of Dynamical, Nondynamical and Dispersion Correlations. Presented at the 47th Sanibel Symposium, St. Simon's Island, USA (2007).
2. E. R. Johnson and A. D. Becke, Van der Waals Interactions from the Exchange Hole Dipole Moment. Presented at the 6th Canadian Computational Chemistry Conference, University of British Columbia (2006).

3. E. R. Johnson and A. D. Becke, Van der Waals Interactions from the Exchange Hole Dipole Moment. Presented at the 46th Sanibel Symposium, St. Simon's Island, USA (2006).
4. E. R. Johnson, A. D. Becke, and G. A. DiLabio, Applicability of Density Functional Theory for Structures and Binding Energies of van der Waals Complexes. Presented at the CECAM workshop on van der Waals Forces and Density Functional Theory, Lyon, France (2005).
5. E. R. Johnson and G. A. DiLabio, Effective Computational Modeling of Large Chemical Systems Using Quantum Capping Potentials. Presented at the 88th Canadian Chemistry Conference, Saskatoon (2005).
6. E. R. Johnson and A. D. Becke, A Post-Hartree-Fock Model of Intermolecular Interactions. Presented at the 45th Sanibel Symposium, St. Simon's Island, USA (2005).
7. E. R. Johnson, O. J. Clarkin, and G. A. DiLabio, Density Functional Theory based Model Calculations for Accurate Bond Dissociation Enthalpies: A Single Approach for X-H, X-X, and X-Y (X, Y = C, N, O, S, Halogen) Bonds. Presented at the 86th Canadian Chemistry Conference, Ottawa (2003).
8. E. R. Johnson, O. J. Clarkin, and G. A. DiLabio, Density Functional Theory based Model Calculations for Accurate Bond Dissociation Enthalpies: A Single Approach for X-H, X-X, and X-Y (X, Y = C, N, O, S, Halogen) Bonds. Presented at the 5th Canadian Computational Chemistry Conference, University of Toronto (2003).
9. E. R. Johnson, P. Kruse, R. A. Wolkow, and G. A. DiLabio, A Theoretical and Experimental Study of Self-Directed Molecular Line Growth of Vinylferrocene on the H-Si(100) Surface. Presented at the Physical Organic Mini-Symposium, University of Windsor (2002).