ROBERT A. DISTASIO JR., PH.D.

Assistant Professor | Department of Chemistry and Chemical Biology | Cornell University
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Education

Princeton University

Postdoctoral Research Associate (2009–2015)
Roberto Car, Research Advisor

University of California, Berkeley

Ph.D. Theoretical Chemistry (2004–2009)
Martin Head-Gordon, Research/Thesis Advisor

California Institute of Technology

Graduate Student (2003–2004)
William A. Goddard III, Research Advisor

Portland State University

B.S. Chemistry and Biology (1999–2003)
Graduated *summa cum laude*
Carl C. Wamser, Research Advisor

Academic Experience

Cornell University — July 1, 2015–present

Assistant Professor

Research: Research in the DiStasio group focuses on the development, implementation, and application of novel methodologies that extend the frontiers of electronic structure theory in complex condensed-phase environments. By utilizing the computational techniques of quantum and statistical mechanics, the DiStasio group seeks to address challenging problems in theoretical chemistry and further our understanding of fundamental systems and processes of importance throughout all disciplines of chemistry, ranging from organic/inorganic chemistry (*i.e.*, catalyst design, solvation/solvent effects) to biochemistry (*i.e.*, stability, structure, and function of proteins, enzymes, and DNA/RNA, drug discovery) and materials science (*i.e.*, molecular crystal polymorphism, forward and inverse design of novel materials).

Teaching: Teaching assignments include instructor for Mathematical Methods of Physical Chemistry (CHEM 7870; Fall 2015, 2017, 2018, 2019), a graduate-level course which prepares students for research in Experimental and Theoretical Physical Chemistry, and Honors Physical Chemistry II (CHEM 3900; Spring 2017, 2018, 2019), an advanced undergraduate-level course in Statistical Mechanics, Classical Thermodynamics, Equilibrium Concepts, and Chemical Kinetics.

Advising: Voluntary instructor for Arts and Sciences Advising Seminar (AS 1102; Fall 2018), a pilot program that provides extended advising and mentoring to a group of 8-10 incoming first-year undergraduates.

Princeton University — 2009–2015

Postdoctoral Research Associate

Research: Research projects include the development and implementation of a theoretical and algorithmic framework for performing path-integral ab initio molecular dynamics (PI-AIMD) simulations of condensed-phase molecular systems based on van der Waals (vdW) inclusive hybrid Density Functional Theory (DFT), with applications to liquid water, aqueous ionic solutions, and molecular crystals; theoretical development of many-body vdW/dispersion corrections in DFT; theoretical development of inverse statistical mechanics approaches, with applications to the design of spin systems and materials.

Teaching: Teaching assignments included co-instructor for undergraduate-level Physical Chemistry/Quantum Mechanics (with Annabella Selloni), guest lecturer for graduate-level Advanced Quantum Mechanics (for Roberto Car), guest lecturer for graduate-level Monte Carlo and Molecular Dynamics Simulation in Statistical Physics and Materials Science (for Roberto Car).

University of California, Berkeley 2004–2009

Graduate Student / Research Assistant / Teaching Assistant

Thesis: Local and Canonical Approximations in Møller-Plesset Perturbation Theory with Applications to Dispersion Interactions.

Research: Research projects included the theoretical development and implementation of local approximations to second-order Møller-Plesset perturbation (MP2) theory, analytical gradient theory within resolution-of-the-identity MP2 (RI-MP2) theory, spin-component scaled MP2 models (SCS-MP2, SCS(MI)-MP2), approximations to three-body correlation in perturbation (MP4) and coupled-cluster (CCSD(T)) theories, dual-basis approximations to Hartree-Fock (DB-HF) and Density Functional Theory (DB-DFT), development of double-hybrid density functionals (B2-P3LYP), chemical applications to polypeptide relative conformational energetics (alanine tetrapeptide) and dispersion interactions in the benzene and fullerene dimers.

Teaching: Teaching assignments included head teaching assistant for undergraduate-level General Chemistry (with Richard Saykally), head teaching assistant for undergraduate-level General Chemistry (with Alex Pines), teaching assistant for graduate-level Advanced Quantum Mechanics (with Martin Head-Gordon).

California Institute of Technology 2003–2004

Graduate Student / Research Assistant / Teaching Assistant

Research: Research projects included the computational (DFT) design of transition-metal catalysts (rhenium-based) to be utilized in the conversion of methane to methanol, mechanistic investigation of the deactivation pathways of methylrhenium trioxide (MTO).

Graduate Coursework (4.0/4.0 Overall GPA): Graduate coursework included Advanced Quantum Mechanics I (Grade: 4.0, with Aron Kuppermann), The Nature of the Chemical Bond (Grade: 4.0, with William A. Goddard III), Advanced Quantum Mechanics II (Grade: 4.0, with B. Vincent McKoy), Statistical Mechanics (Grade: 4.0, with Zhen-Gang Wang), and Advanced Quantum Mechanics III (Grade: 4.0, with Daniel P. Weitekamp).

Teaching: Teaching assignments included head teaching assistant for undergraduate-level Quantum Chemistry (with B. Vincent McKoy) and teaching assistant for undergraduate-level General Chemistry (with James R. Heath and David W. MacMillan).

Portland State University 1999–2003

Undergraduate Student / Research Assistant / Teaching Assistant

Research: Research projects included the synthesis of several *p*-substituted tetraphenylporphyrins, experimental and theoretical investigation of the isothermal adsorption of these porphyrins onto sintered nanoparticulate titanium dioxide (TiO2) electrodes for use in alternative solar cells.

Undergraduate Coursework (3.96/4.0 Overall GPA): Undergraduate coursework in Chemistry included General Chemistry, Organic Chemistry, Analytical Chemistry, Instrumental Analysis, Spectrometric Analysis, Inorganic Chemistry, Biochemistry, Physical Chemistry, Computational Chemistry, Molecular Modeling, and all corresponding laboratories; Undergraduate coursework in Physics and Mathematics included General Physics, Modern Physics, Quantum Mechanics, Calculus, Applied Differential Equations, Linear Algebra, Group Theory, Numerical Analysis, and all corresponding laboratories; Undergraduate coursework in Biology included General Biology, Genetics, Ecology, Molecular Biology, Molecular Cell Physiology, Microbiology, Immunology/Serology, Virology, and all corresponding laboratories.

Teaching: Teaching assignments included teaching assistant for undergraduate-level General Chemistry Laboratory (six quarters with Gwen P. Shusterman), workshop/peer leader for undergraduate-level Organic Chemistry (nine quarters with Carl C. Wamser).

University of Georgia/Center for Computational and Quantum Chemistry Summer 2002

Summer Undergraduate Research Fellow

Research: Research projects included the computational (DFT) investigation of adiabatic electron affinities, singlet-triplet gaps, and local aromaticity in pentalene-annulated polycyclic aromatic hydrocarbons. Attended the CCQC summer lectures series on group theory, geometry optimization, vibrational frequency analysis, self-consistent field and Hartree-Fock theory, Density Functional Theory, Møller-Plesset perturbation theory, coupled cluster theory, configuration interaction, and relativistic quantum chemistry.

PUBLICATIONS (* denotes corresponding author(s))

61. E. G. Fuemmeler, A. Damle, and **R. A. DiStasio Jr.***, *Selected Columns of the Density Matrix in an Atomic Orbital Basis I: An Intrinsic and Non-Iterative Orbital Localization Scheme for the Occupied Space.* J. Chem. Theory Comput. (*in press*).

60. L. Song, N. Fu, B. G. Ernst, W. H. Lee, M. O. Frederick, **R. A. DiStasio Jr.***, and S. Lin*, *Dual Electrocatalysis Enables Enantioselective Hydrocyanation of Conjugated Alkenes.* Nat. Chem. **12**, 747 (2020).

59. B. G. Ernst, K. U. Lao, A. G. Sullivan, and **R. A. DiStasio Jr.***, *Attracting Opposites: Promiscuous Ion-π Binding in the Nucleobases.* J. Phys. Chem. A **124**, 4128 (2020).

58. H.-Y. Ko, J. Jia, B. Santra, X. Wu, R. Car, and **R. A. DiStasio Jr.***, *Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics. 1. Theory, Algorithm, and Performance.* J. Chem. Theory Comput. **16**, 3757 (2020).

57. Y. Vidavsky, M. R. Buche, Z. M. Sparrow, X. Zhang, S. J. Yang, **R. A. DiStasio Jr.***, and M. N. Silberstein*, *Tuning the Mechanical Properties of Metallopolymers via Ligand Interactions: A Combined Experimental and Theoretical Study.* Macromolecules **53**, 2021 (2020).

56. T. Suh, Y. Yang, P. Zhao, K. U. Lao, H.-Y. Ko, J. Wong, **R. A. DiStasio Jr.***, and J. R. Engstrom*, *Competitive Adsorption as a Route to Area-Selective Deposition.* ACS Appl. Mater. Interfaces **12**, 9989 (2020).

55. H.-Y. Ko, L. Zhang, B. Santra, H. Wang, W. E, **R. A. DiStasio Jr.**, and R. Car, *Isotope Effects in Liquid Water via Deep Potential Molecular Dynamics.* Mol. Phys. **117**, 3269 (2019).

54. Y. Yang, K. U. Lao, D. M. Wilkins, A. Grisafi, M. Ceriotti*, and **R. A. DiStasio Jr.***, *Quantum Mechanical Static Dipole Polarizabilities in the QM7b and AlphaML Showcase Databases.* Sci. Data **6**, 152 (2019).

53. D. M. Wilkins, A. Grisafi, Y. Yang, K. U. Lao, **R. A. DiStasio Jr.***, and M. Ceriotti*, *Accurate Molecular Polarizabilities with Coupled-Cluster Theory and Machine Learning.* Proc. Natl. Acad. Sci. USA **116**, 3401 (2019).

52. J. Hoja, H.-Y. Ko, M. A. Neumann, R. Car, **R. A. DiStasio Jr.**, and A. Tkatchenko, *Reliable and Practical Computational Description of Molecular Crystal Polymorphs.* Sci. Adv. **5**, eaau3338 (2019).

51. Y. Yang, K. U. Lao, and **R. A. DiStasio Jr.***, *Influence of Pore Size on the van der Waals Interaction in Two-Dimensional Molecules and Materials.* Phys. Rev. Lett. **122**, 026001 (2019).

50. K. U. Lao, J. Jia, R. Maitra, and **R. A. DiStasio Jr.***, *On the Geometric Dependence of the Molecular Dipole Polarizability in Water: A Benchmark Study of Higher-Order Electron Correlation, Basis Set Incompleteness Error, Core Electron Effects, and Zero-Point Vibrational Contributions.* J. Chem. Phys. **149**, 204303 (2018).

49. X. Yu, J. Jia, S. Xu, M. J. Sanford, R. K. Ramakrishnan, S. I. Nazarenko, T. R. Hoye, G. W. Coates*, and **R. A. DiStasio Jr.***, *Unraveling Substituent Effects on the Glass Transition Temperatures of Biorenewable Polyesters.* Nat. Commun. **9**, 2880 (2018).

48. T. Bereau, **R. A. DiStasio Jr.**, A. Tkatchenko, and O. A. von Lilienfeld, *Non-covalent Interactions across Organic and Biological Subsets of Chemical Space: Physics-Based Potentials Parameterized from Machine Learning.* J. Chem. Phys. **148**, 241706b (2018).

47. H.-Y. Ko, **R. A. DiStasio Jr.**, B. Santra, and R. Car, *Thermal Expansion in Dispersion-Bound Molecular Crystals.* Phys. Rev. Materials **2**, 055603 (2018).

46. I. Poltavsky, **R. A. DiStasio Jr.**, and A. Tkatchenko, *Perturbed Path Integrals in Imaginary Time: Efficiently Modeling Nuclear Quantum Effects in Molecules and Materials.* J. Chem. Phys. **148**, 102325 (2018).

45. M. Chen, L. Zheng, B. Santra, H.-Y. Ko, **R. A. DiStasio Jr.**, M. L. Klein, R. Car, and X. Wu, *Hydroxide Diffuses Slower than Hydronium in Water Because its Solvated Structure Inhibits Correlated Proton Transfer.* Nat. Chem. **10**, 413 (2018).

44. D. T. Gentekos, J. Jia, E. S. Tirado, K. P. Barteau, **R. A. DiStasio Jr.***, and B. P. Fors*, *Exploiting Molecular Weight Distribution Shape to Tune Domain Spacing in Block Copolymer Thin Films.* J. Am. Chem. Soc. **140**, 4639 (2018).

43. S. Xie, L. Tu, Y. Han, L. Huang, K. Kang, K. U. Lao, P. Poddar, C. Park, D. A. Muller, **R. A. DiStasio Jr.**, and J. Park, *Coherent, Atomically Thin Transition-Metal Dichalcogenide Superlattices with Engineered Strain.* Science **359**, 1131 (2018).

42. **R. A. DiStasio Jr.**, G. Zhang, F. H. Stillinger, and S. Torquato *Rational Design of Stealthy Hyperuniform Two-Phase Media with Tunable Order.* Phys. Rev. E **97**, 023311 (2018).

41. P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. Buongiorno Nardelli, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. Carnimeo, A. Dal Corso, S. De Gironcoli, P. Delugas, **R. A. DiStasio Jr.**, A. Ferretti, A. Floris, G. Fratesi, G. Fugallo, R. Gebauer, U. Gerstmann, F. Giustino, T. Gorni, J. Jia, M. Kawamura, H.-Y. Ko, A. Kokalj, E. Küçükbenli, M. Lazzeri, M. Marsili, N. Marzari, F. Mauri, N. L. Nguyen, H. V. Nguyen, A. Otero-De-La-Roza, L. Paulatto, S. Poncé, D. Rocca, R. Sabatini, B. Santra, M. Schlipf, A. P. Seitsonen, A. Smogunov, I. Timrov, T. Thonhauser, P. Umari, N. Vast, X. Wu, and S. Baroni, *Advanced Capabilities for Materials Modeling with Quantum ESPRESSO.* J. Phys.: Condens. Matter **29**, 465901 (2017).

40. A. Genova, D. Ceresoli, A. Krishtal, O. Andreussi, **R. A. DiStasio Jr.**, and M. Pavanello, *eQE: An Open-Source Density Functional Embedding Theory Code for the Condensed Phase.* Int. J. Quantum Chem. **117**, e25401 (2017).

39. J. Hermann, **R. A. DiStasio Jr.***, and A. Tkatchenko*, *First-Principles Models for van der Waals Interactions in Molecules: Concepts, Theory, and Applications.* Chem. Rev. (Special Issue on Non-Covalent Interactions) **117**, 4714 (2017).

38. A. M. Reilly, R. I. Cooper, C. S. Adjiman, S. Bhattacharya, A. D. Boese, J. G. Brandenburg, P. J. Bygrave, R. Bylsma, J. E. Campbell, R. Car, D. H. Case, R. Chadha, J. C. Cole, K. Cosburn, H. M. Cuppen, F. Curtis, G. M. Day, **R. A. DiStasio Jr.**, A. Dzyabchenko, B. P. van Eijck, D. M. Elking, J. A. van den Ende, J. C. Facelli, M. B. Ferraro, L. Fusti-Molnar, C.-A. Gatsiou, T. S. Gee, R. de Gelder, L. M. Ghiringhelli, H. Goto, S. Grimme, R. Guo, D. W. M. Hofmann, J. Hoja, R. K. Hylton, L. Iuzzolino, W. Jankiewicz, D. T. de Jong, J. Kendrick, N. J. J. de Klerk, H.-Y. Ko, L. N. Kuleshova, X. Li, S. Lohani, F. J. J. Leusen, A. M. Lund, J. Lv, Y. Ma, N. Marom, A. E. Masunov, P. McCabe, D. P. McMahon, H. Meekes, M. P. Metz, A. J. Misquitta, S. Mohamed, B. Monserrat, R. J. Needs, M. A. Neumann, J. Nyman, S. Obata, H. Oberhofer, A. R. Oganov, A. M. Orendt, G. I. Pagola, C. C. Pantelides, C. J. Pickard, R. Podeszwa, L. S. Price, S. L. Price, A. Pulido, M. G. Read, K. Reuter, E. Schneider, C. Schober, G. P. Shields, P. Singh, I. J. Sugden, K. Szalewicz, C. R. Taylor, A. Tkatchenko, M. E. Tuckerman, F. Vacarro, M. Vasileiadis, A. Vazquez-Mayagoitia, L. Vogt, Y. Wang, R. E. Watson, G. A. de Wijs, J. Yang, Q. Zhu, and C. R. Groom, *Report on the Sixth Blind Test of Organic Crystal Structure Prediction Methods.* Acta Cryst. **B72**, 439 (2016).

37. A. Ambrosetti, N. Ferri, **R. A. DiStasio Jr.***, and A. Tkatchenko*, *Wavelike Charge Density Fluctuations and van der Waals Interactions at the Nanoscale.* Science **351**, 1171 (2016).

36. E. Chertkov, **R. A. DiStasio Jr.**, G. Zhang, R. Car, and S. Torquato, *Inverse Design of Disordered Stealthy Hyperuniform Spin Chains.* Phys. Rev. B (Editors' Suggestion) **93**, 064201 (2016).

35. M. A. Blood-Forsythe, T. Markovich, **R. A. DiStasio Jr.**, R. Car, and A. Aspuru-Guzik, *Analytical Nuclear Gradients for the Range-Separated Many-Body Dispersion Model of Noncovalent Interactions.* Chem. Sci. **7**, 1712 (2016).

B.C. (Before Cornell)

34. A. Bankura, B. Santra, **R. A. DiStasio Jr.**, C. W. Swartz, M. L. Klein, and X. Wu, *A Systematic Study of Chloride Ion Solvation in Water Using van der Waals Inclusive Hybrid Density Functional Theory.* Mol. Phys. (Jean-Pierre Hansen Special Issue) **113**, 2842 (2015).

33. B. Santra, **R. A. DiStasio Jr.**, F. Martelli, and R. Car, *Local Structure Analysis in Ab Initio Liquid Water.* Mol. Phys. (Jean-Pierre Hansen Special Issue) **113**, 2829 (2015).

32. Y. Mei, A. C. Simmonett, F. C. Pickard IV, **R. A. DiStasio Jr.**, B. R. Brooks, and Y. Shao, *Numerical Study on the Partitioning of the Molecular Polarizability into Fluctuating Charge and Induced Atomic Dipole Contributions.* J. Phys. Chem. A **119**, 5865 (2015).

31. N. Ferri, **R. A. DiStasio Jr.**, A. Ambrosetti, R. Car, and A. Tkatchenko, *Electronic Properties of Molecules and Surfaces with a Self-Consistent Interatomic van der Waals Density Functional.* Phys. Rev. Lett. **114**, 176802 (2015).

30. **R. A. DiStasio Jr.**, B. Santra, Z. Li, X. Wu, and R. Car, *The Individual and Collective Effects of Exact Exchange and Dispersion Interactions on the Ab Initio Structure of Liquid Water.* J. Chem. Phys. **141**, 084502 (2014).

29. Y. Shao, Z. Gan, E. Epifanovsky, A. T. Gilbert, M. Wormit, J. Kussmann, A. W. Lange, A. Behn, J. Deng, X. Feng, D. Ghosh, M. Goldey, P. R. Horn, L. D. Jacobson, I. Kaliman, R. Z. Khaliullin, T. Ku, A. Landau, J. Liu, E. I. Proynov, Y. M. Rhee, R. M. Richard, M. A. Rohrdanz, R. P. Steele, E. J. Sundstrom, H. L. Woodcock, P. M. Zimmerman, D. Zuev, B. Albrecht, E. Alguire, B. Austin, G. J. O. Beran, Y. A. Bernard, E. Berquist, K. Brandhorst, K. B. Bravaya, S. T. Brown,

D. Casanova, C.-M. Chang, Y. Chen, S. H. Chien, K. D. Closser, D. L. Crittenden, M. Diedenhofen, **R. A. DiStasio Jr.**, H. Do, A. D. Dutoi, R. G. Edgar, S. Fatehi, L. Fusti-Molnar, A. Ghysels, A. Golubeva-Zadorozhnaya, J. Gomes, M. W. Hanson-Heine, P. H. Harbach, A. W. Hauser, E. G. Hohenstein, Z. C. Holden, T.-C. Jagau, H. Ji, B. Kaduk, K. Khistyaev, J. Kim, J. Kim, R. A. King, P. Klunzinger, D. Kosenkov, T. Kowalczyk, C. M. Krauter, K. U. Lao, A. Laurent, K. V. Lawler, S. V. Levchenko, C. Y. Lin, F. Liu, E. Livshits, R. C. Lochan, A. Luenser, P. Manohar, S. F. Manzer, S.-P. Mao, N. Mardirossian, A. V. Marenich, S. A. Maurer, N. J. Mayhall, E. Neuscamman, C. M. Oana, R. Olivares-Amaya, D. P. O'Neill, J. A. Parkhill, T. M. Perrine, R. Peverati, A. Prociuk, D. R. Rehn, E. Rosta, N. J. Russ, S. M. Sharada, S. Sharma, D. W. Small, A. Sodt, T. Stein, D. Stck, Y.-C. Su, A. J. W. Thom, T. Tsuchimochi, V. Vanovschi, L. Vogt, O. Vydrov, T. Wang, M. A. Watson, J. Wenzel, A. White, C. F. Williams, J. Yang, S. Yeganeh, S. R. Yost, Z.-Q. You, I. Y. Zhang, X. Zhang, Y. Zhao, B. R. Brooks, G. K. L. Chan, D. M. Chipman, C. J. Cramer, W. A. Goddard III, M. S. Gordon, W. J. Hehre, A. Klamt, H. F. Schaefer III, M. W. Schmidt, C. D. Sherrill, D. G. Truhlar, A. Warshel, X. Xu, A. Aspuru-Guzik, R. Baer, A. T. Bell, N. A. Besley, J.-D. Chai, A. Dreuw, B. D. Dunietz, T. R. Furlani, S. R. Gwaltney, C.-P. Hsu, Y. Jung, J. Kong, D. S. Lambrecht, W. Liang, C. Ochsenfeld, V. A. Rassolov, L. V. Slipchenko, J. E. Subotnik, T. Van Voorhis, J. M. Herbert, A. I. Krylov, P. M. Gill, and M. Head-Gordon, *Advances in Molecular Quantum Chemistry Contained in the Q-Chem 4 Program Package.* Mol. Phys. **113**, 184 (2014).

28. **R. A. DiStasio Jr.**, V. V. Gobre, and A. Tkatchenko, *Many-Body van der Waals Interactions in Molecules and Condensed Matter.* J. Phys.: Condens. Matter **26**, 213202 (2014).

27. M. Goldey, **R. A. DiStasio Jr.**, Y. Shao, and M. Head-Gordon, *Shared Memory Multiprocessing Implementation of Resolution-of-the-Identity Second-Order Møller-Plesset Perturbation Theory with Attenuated and Unattenuated Results for Intermolecular Interactions between Large Molecules.* Mol. Phys. (Invited Article) **112**, 836 (2014).

26. A. Ambrosetti, D. Alfé, **R. A. DiStasio Jr.**, and A. Tkatchenko, *Hard Numbers for Large Molecules: Toward Exact Energetics for Supramolecular Systems.* J. Phys. Chem. Lett. **5**, 849 (2014).

25. A. Ambrosetti, A. M. Reilly, **R. A. DiStasio Jr.**, and A. Tkatchenko, *Long-Range Correlation Energy Calculated from Coupled Atomic Response Functions.* J. Chem. Phys. (Invited Article) **140**, 18A508 (2014).

24. **R. A. DiStasio Jr.**, É. Marcotte, R. Car, F. Stillinger, and S. Torquato, *Designer Spin Systems via Inverse Statistical Mechanics.* Phys. Rev. B (Editors' Suggestion) **88**, 134104 (2013).

23. É. Marcotte, **R. A. DiStasio Jr.**, F. Stillinger, and S. Torquato, *Designer Spin Systems via Inverse Statistical Mechanics. II. Ground-State Enumeration and Classification.* Phys. Rev. B **88**, 184432 (2013).

22. N. Marom, **R. A. DiStasio Jr.**, V. Attala, S. Levchenko, A. M. Reilly, J. R. Chelikowsky, L. Leiserowitz, and A. Tkatchenko, *Many-Body Dispersion Interactions in Molecular Crystal Polymorphism.* Angew. Chem. Int. Ed. **52**, 6629 (2013).

21. A. Tkatchenko, A. Ambrosetti, and **R. A. DiStasio Jr.**, *Interatomic Methods for the Dispersion Energy Derived from the Adiabatic Connection Fluctuation-Dissipation Theorem.* J. Chem. Phys. **138**, 074106 (2013).

20. **R. A. DiStasio Jr.**, V. V. Gobre, and A. Tkatchenko, *Many-Body van der Waals Interactions in Biology, Chemistry, and Physics.* Ψ_k Newsletter (Scientific Highlight of the Month) **114**, 47 (2012).

19. **R. A. DiStasio Jr.**, O. A. von Lilienfeld, and A. Tkatchenko, *Collective Many-Body van der Waals Interactions in Molecular Systems.* Proc. Natl. Acad. Sci. USA **109**, 14791 (2012).

18. A. Tkatchenko, **R. A. DiStasio Jr.**, R. Car, and M. Scheffler, *Accurate and Efficient Method for Many-Body van der Waals Interactions.* Phys. Rev. Lett. **108**, 236402 (2012).

17. J. W. Ponder, C. Wu, P. Ren, V. S. Pande, J. D. Chodera, M. J. Schnieders, I. Haque, D. L. Mobley, D. S. Lambrecht, **R. A. DiStasio Jr.**, M. Head-Gordon, G. N. I. Clark, M. E. Johnson, and T. Head-Gordon, *Current Status of the AMOEBA Polarizable Force Field.* J. Phys. Chem. B (Feature Article) **114**, 2549 (2010).

16. R. P. Steele, **R. A. DiStasio Jr.**, M. Head-Gordon, Y. Li, and G. Galli, *The 1,4-phenylenediisocyanide Dimer: Gas-Phase Properties and Insights into Organic Self-Assembled Monolayers.* Phys. Chem. Chem. Phys. **12**, 82 (2010).

15. A. Tkatchenko, **R. A. DiStasio Jr.**, M. Head-Gordon, and M. Scheffler, *Dispersion-Corrected Møller-Plesset Second-Order Perturbation Theory.* J. Chem. Phys. **131**, 094106 (2009).

14. R. P. Steele, **R. A. DiStasio Jr.**, and M. Head-Gordon, *Non-Covalent Interactions with Dual-Basis Methods: Pairings for Augmented Basis Sets.* J. Chem. Theory Comput. **5**, 1560 (2009).

13. T. Benighaus, **R. A. DiStasio Jr.**, R. C. Lochan, J.-D. Chai, and M. Head-Gordon, *Semiempirical Double-Hybrid Density Functional with Improved Description of Long-Range Correlation.* J. Phys. Chem. A **112**, 2702 (2008).

12. J. M. Gonzales, **R. A. DiStasio Jr.**, R. A. Periana, W. A. Goddard III, and J. Oxgaard, *Methylrhenium Trioxide Revisited: Mechanisms for Nonredox Oxygen Insertion in an M-CH_3 Bond.* J. Amer. Chem. Soc. **129**, 15794 (2007).

11. **R. A. DiStasio Jr.**, R. P. Steele, and M. Head-Gordon, *The Analytical Gradient of Dual-Basis Resolution-of-the-Identity Second-Order Møller-Plesset Perturbation Theory.* Mol. Phys. (Peter Pulay Special Issue) **105**, 2731 (2007).

10. **R. A. DiStasio Jr.** and M. Head-Gordon, *Optimized Spin-Component Scaled Second-Order Møller-Plesset Perturbation Theory for Intermolecular Interaction Energies.* Mol. Phys. **105**, 1073 (2007).

9. **R. A. DiStasio Jr.**, G. von Helden, R. P. Steele, and M. Head-Gordon, *On the T-Shaped Structures of the Benzene Dimer.* Chem. Phys. Lett. **437**, 277 (2007).

8. E. A. Glascoe, M. F. Kling, J. E. Shanoski, **R. A. DiStasio Jr.**, C. K. Payne, B. V. Mork, T. D. Tilley, and C. B. Harris, *Photoinduced β-Hydrogen Elimination and Radical Formation with $CpW(CO)_3(CH_2CH_3)$: Ultrafast IR and DFT Studies.* Organometallics **26**, 1424 (2007).

7. **R. A. DiStasio Jr.**, R. P. Steele, Y. M. Rhee, Y. Shao, and M. Head-Gordon, *An Improved Algorithm for Analytical Gradient Evaluation in Resolution-of-the-Identity Second-Order Møller-Plesset Perturbation Theory: Application to Alanine Tetrapeptide Conformational Analysis.* J. Comput. Chem. **28**, 839 (2007).

6. R. P. Steele, Y. Shao, **R. A. DiStasio Jr.**, and M. Head-Gordon, *Dual-Basis Analytic Gradients. I. Self-Consistent Field Theory.* J. Phys. Chem. A **110**, 13915 (2006).

5. Y. Shao, L. Fusti-Molnar, Y. Jung, J. Kussmann, C. Ochsenfeld, S. T. Brown, A. T. B. Gilbert, L. V. Slipchenko, S. V. Levchenko, D. P. O'Neill, **R. A. DiStasio Jr.**, R. C. Lochan, T. Wang, G. J. O. Beran, N. A. Besley, J. M. Herbert, C. Y. Lin, T. Van Voorhis, S. H. Chien, A. Sodt, R. P. Steele, V. A. Rassolov, P. E. Maslen, P. P. Korambath, R. D. Adamson, B. Austin, J. Baker, E. F. C. Byrd, H. Dachsel, R. J. Doerksen, A. Dreuw, B. D. Dunietz, A. D. Dutoi, T. R. Furlani, S. R. Gwaltney, A. Heyden, S. Hirata, C. P. Hsu, G. Kedziora, R. Z. Khalliulin, P. Klunzinger, A. M. Lee, M. S. Lee, W. Liang, I. Lotan, N. Nair, B. Peters, E. I. Proynov, P. A. Pieniazek, Y. M. Rhee, J. Ritchie, E. Rosta, C. D. Sherrill, A. C. Simmonett, J. E. Subotnik, H. L. Woodcock III, W. Zhang, A. T. Bell, A. K. Chakraborty, D. M. Chipman, F. J. Keil, A. Warshel, W. J. Hehre, H. F. Schaefer III, J. Kong, A. I. Krylov, P. M. W. Gill, and M. Head-Gordon, *Q-Chem 3.0: Advances in Methods and Algorithms in a Modern Quantum Chemistry Program Package.* Phys. Chem. Chem. Phys. **8**, 3172 (2006).

4. R. P. Steele, **R. A. DiStasio Jr.**, Y. Shao, J. Kong, and M. Head-Gordon, *Dual-Basis Second-Order Møller-Plesset Perturbation Theory: A Reduced Cost Reference for Correlation Calculations.* J. Chem. Phys. **125**, 074108 (2006).

3. Y. M. Rhee, **R. A. DiStasio Jr.**, R. C. Lochan, and M. Head-Gordon, *Analytical Gradient of Restricted Second-Order Møller-Plesset Correlation Energy with the Resolution-of-the-Identity Approximation, Applied to the TCNE Dimer Anion Complex.* Chem. Phys. Lett. **426**, 197 (2006).

2. **R. A. DiStasio Jr.**, Y. Jung, and M. Head-Gordon, *A Resolution-of-the-Identity Implementation of the Local Triatomics-in-Molecules Model for Second-Order Møller-Plesset Perturbation Theory with Application to Alanine Tetrapeptide Conformational Energies.* J. Chem. Theory Comput. **1**, 862 (2005).

1. J. A. Smith, **R. A. DiStasio Jr.**, N. A. Hannah, R. W. Winter, T. J. R. Weakley, G. L. Gard, and S. B. Rananavare, *SF_5-Terminated Fluorinated Schiff Base Liquid Crystals.* J. Phys. Chem. B **108**, 19940 (2004).

Plenary Talks

2. "First Principles Approaches for Intermolecular Interactions: From Gas-Phase Dimers to Liquid Water and Molecular Crystal Polymorphism", Portland State of Mind, 7th Annual Alumni Seminar and Graduate Research Symposium: Portland State University, Portland, OR, 2019.

1. "First Principles Approaches for Intermolecular Interactions: From Gas-Phase Dimers to Liquid Water and Molecular Crystal Polymorphism", 10^{th} International Conference on Computational Physics (ICCP10): Macao SAR, China, 2017.

Invited Talks

54. "DFT and Beyond: Benchmark Data for Next-Generation Machine Learning of Intra- and Inter-Molecular Interactions", Molecular Simulation with Machine Learning Workshop, Princeton, NJ, 2020 (virtual).

53. "DFT and Beyond: Benchmark Data for Next-Generation Machine Learning of Intra- and Inter-Molecular Interactions", American Chemical Society National Meeting: San Francisco, CA, 2020 (virtual).

52. "On the Higher-Order Static Polarizabilities and Dispersion Coefficients of the Fullerenes: An *Ab Initio* Study", Telluride Science Research Center (TSRC) Workshop, *Many-Body Interactions: From Quantum Mechanics to Force Fields*: Telluride, CO, 2020 (virtual).

51. "Exploiting Orbital Locality in Real Space to Enable Large-Scale Condensed-Phase *Ab Initio* Molecular Dynamics with Hybrid Density Functional Theory", American Physical Society March Meeting: Denver, CO, 2020 (cancelled).

50. "Rational Solid Form Design Summit Panel on Crystal Structure Prediction", 2019 Rational Solid Form Design Summit: Boston, MA, 2019.

49. "Thermal Expansion in Dispersion-Bound Molecular Crystals", Telluride Science Research Center (TSRC) Workshop, *Quantum Effects in Condensed-Phase Systems*: Telluride, CO, 2019.

48. "Attracting Opposites: Promiscuous Ion-pi Binding in the Nucleobases", Telluride Science Research Center (TSRC) Workshop, *Intermolecular Interactions: New Challenges for Ab Initio Theory*: Telluride, CO, 2019.

47. "Attacking the Strong and Weak Scaling Limits in Linear Scaling Hybrid Density Functional Theory", Hong Kong University of Science and Technology—Institute for Advanced Study Program, *Quantum Simulations: From Chemistry to Materials Science*: Hong Kong, 2018.

46. "Attacking the Strong and Weak Scaling Limits in Linear Scaling Hybrid Density Functional Theory", Center for Computational Materials, Institute of Computational Engineering and Sciences, University of Texas at Austin Workshop, *Planning the Next Generation of Real-Space Electronic Structure Computer Codes*: Austin, TX, 2018.

45. "Attacking the Strong Scaling Limit in Linear Scaling Hybrid Density Functional Theory", 256^{th} American Chemical Society National Meeting: Boston, MA, 2018.

44. "Influence of Pore Size on the van der Waals Interaction in Two-Dimensional Molecules and Materials", Telluride Science Research Center (TSRC) Workshop, *Many-Body Interactions: From Quantum Mechanics to Force Fields*: Telluride, CO, 2018.

43. "Benchmark Estimates of the Multipole Polarizabilities of Atoms and Molecules", CECAM Workshop, *Machine Learning at Interfaces*, Ecole Polytechnique Fédérale de Lausanne (EPFL): Lausanne, Switzerland, 2018.

42. "Attacking the Strong Scaling Limit in Condensed-Phase Hybrid DFT", Electronic Structure (ES'18) and Penn Conference in Theoretical Chemistry (PCTC'18): Philadelphia, PA, 2018.

41. "The Dipole Polarizability of a Condensed-Phase Water Molecule", Syracuse University: Syracuse, NY, 2018.

40. "Enabling Large-Scale Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics in the Condensed Phase", CECAM Workshop, *Expeditious Methods in Electronic Structure Theory and Many Body Techniques*, Tel Aviv University: Tel Aviv, Israel, 2017.

39. "The Dipole Polarizability of a Condensed-Phased Water Molecule", Weizmann Institute of Science: Rehovot, Israel, 2017.

38. "Benchmark Estimates of the Multipole Polarizabilities of Atoms and Molecules", NIPS Workshop, *Machine Learning for Molecules and Materials*: Long Beach, CA, 2017.

37. "The Dipole Polarizability of a Condensed-Phased Water Molecule", CPMD 2017: Tsukuba, Japan, 2017.

36. "Enabling Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics for Large-Scale Condensed-Phase Systems", 254^{th} American Chemical Society National Meeting: Washington, DC, 2017.

35. "Enabling Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics for Large-Scale Condensed-Phase Systems", MolSSI Interoperability Workshop: Blacksburg, VA, 2017.

34. "Enabling Large-Scale Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics in Condensed- Phase Systems", NSF-MolSSI Materials Workshop: Berkeley, CA, 2017.

33. "The Dipole Polarizability of a Condensed-Phase Water Molecule", 10^{th} International Conference on Computational Physics (ICCP10): Macao SAR, China, 2017.

32. "Enabling Large-Scale Hybrid Density Functional Theory in Condensed-Phase Systems", Intel High-Performance Computing Developer Conference: Salt Lake City, UT, 2016.

31. "The Dipole Polarizability of a Condensed-Phase Water Molecule", Institute for Pure and Applied Mathematics: Los Angeles, CA, 2016.

30. "Enabling Large-Scale Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics in Condensed-Phase Systems", Intel Xeon Phi Users' Group (IXPUG) Meeting: Argonne National Laboratory, Lamont, IL, 2016.

29. "The Dipole Polarizability of a Condensed-Phase Water Molecule", 252^{nd} American Chemical Society National Meeting: Philadelphia, PA, 2016.

28. "The Dipole Polarizability of a Condensed-Phase Water Molecule", Argonne National Laboratories: Lemont, IL, 2016.

27. "The Dipole Polarizability of a Condensed-Phase Water Molecule", 9^{th} Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP): Grand Forks, ND, 2016.

26. "The Dipole Polarizability of a Condensed-Phase Water Molecule", Telluride Science Research Center (TSRC) Workshop, *Many-Body Interactions: From Quantum Mechanics to Force Fields*: Telluride, CO, 2016.

25. "First Principles Approaches for Intermolecular Interactions: From Gas-Phase Dimers to Liquid Water and Molecular Crystal Polymorphism", Temple University: Philadelphia, PA, 2016.

24. "First Principles Approaches for Intermolecular Interactions: From Gas-Phase Dimers to Liquid Water and Molecular Crystal Polymorphism", Seoul National University: Seoul, South Korea, 2016.

23. "First Principles Approaches for Intermolecular Interactions: From Gas-Phase Dimers to Liquid Water and Molecular Crystal Polymorphism", Pohang University of Science and Technology: Pohang, South Korea, 2016.

22. "First Principles Approaches for Intermolecular Interactions: From Gas-Phase Dimers to Liquid Water and Molecular Crystal Polymorphism", Korea Advanced Institute of Science and Technology: Daejeon, South Korea, 2016.

21. "Enabling Large-Scale and Systematically-Improvable Density Functional Theory Calculations in Condensed-Phase Systems", Scientific Computing and Numerics (SCAN) Seminar, Cornell University: Ithaca, NY, 2016.

20. "Enabling Large-Scale Hybrid Density Functional Theory Calculations in Condensed-Phase Systems", Intel Xeon Phi Users' Group (IXPUG) Meeting: Berkeley, CA, 2015.

19. "Enabling Large-Scale Hybrid Density Functional Theory Calculations in Condensed-Phase Systems", 250^{th} American Chemical Society National Meeting: Boston, MA, 2015.

18. "Enabling Large-Scale Hybrid Density Functional Theory Calculations in Condensed-Phase Systems", Ψ_k 2015 Conference: San Sebastian, Spain, 2015.

17. "Many-Body Dispersion Interactions in Molecular Materials", American Physical Society March Meeting: San Antonio, TX, 2015.

16. "Enabling Large-Scale Hybrid Density Functional Theory Calculations", Society for Industrial and Applied Mathematics Meeting, Salt Lake City, UT, 2015.

15. "The Microscopic Structure, Equilibrium Density, and Local Environment in Liquid Water", CECAM Workshop, *Addressing Challenges for First-Principles Based Modeling of Molecular Materials*, Ecole Polytechnique Fédérale de Lausanne (EPFL): Lausanne, Switzerland, 2014.

14. "Enabling Highly Accurate Ab Initio Path-Integral Molecular Dynamics: Applications to Liquid Water", Sustainable Software for Chemistry and Materials $(\text{SICM})^2$ Parallel Computing Workshop: New York, NY, 2014.

13. "The Microscopic Structure, Equilibrium Density, and Local Environment of Liquid Water", Harvard University: Cambridge, MA, 2014.

12. "Many-Body van der Waals Interactions: Theory and Applications", Laboratory of Computational Biology, National Institutes of Health (NIH): Bethesda, MD, 2014.

11. "Liquid Water from First Principles: The Importance of Exact Exchange, Dispersion Interactions, and Nuclear Quantum Effects", 3^{rd} Annual Computational Materials and Chemical Sciences Network (CMCSN) Meeting, U. S. Department of Energy (DOE), Office of Basic Energy Sciences: Davis, CA, 2013.

10. "Many-Body van der Waals Interactions: Theory and Applications", University of Pennsylvania: Philadelphia, PA, 2013.

9. "Liquid Water from First Principles: The Importance of Exact Exchange, Dispersion Interactions, and Nuclear Quantum Effects", Fritz-Haber-Institut der Max-Planck-Gesellschaft, Theory Seminar: Berlin, Germany, 2013.

8. "Designer Spin Systems via Inverse Statistical Mechanics", Institute for Pure and Applied Mathematics (IPAM), University of California, Los Angeles: Los Angeles, CA, 2013.

7. "Many-Body van der Waals Interactions: Theory and Applications", CECAM Workshop, *Towards First- Principles Descriptions of vdW Interactions in Complex Materials*, Ecole Polytechnique Fédérale de Lausanne (EPFL): Lausanne, Switzerland, 2012.

6. "Many-Body van der Waals Interactions: Theory and Applications", Telluride Science Research Center (TSRC) Workshop, *Many-Body Interactions: From Quantum Mechanics to Force Fields*: Telluride, CO, 2012.

5. "Designer Spin Systems: Inverse Statistical Mechanics and the Ising Model", Institute for Pure and Applied Mathematics (IPAM), University of California, Los Angeles: Los Angeles, CA, 2012.

4. "An Efficient Real-Space Implementation of the van der Waals Energy and Analytical Forces in Plane-Wave Based DFT and Ab Initio Molecular Dynamics", Computational Surface Science Workshop, University of California, Santa Barbara: Santa Barbara, CA, 2011.

3. "An Efficient Real-Space Implementation of the van der Waals Energy and Analytical Forces in Plane-Wave Based DFT and Car-Parrinello Molecular Dynamics", CPMD 2011 Conference: Barcelona, Spain, 2011.

2. "Quantum Chemical and Semi-Empirical Descriptions of Dispersion Interactions", Fritz-Haber-Institut der Max-Planck-Gesellschaft, Theory Seminar: Berlin, Germany, 2011.

1. "Quantum Chemical and Semi-Empirical Descriptions of Dispersion Interactions", Thiel Group Seminar, Max-Planck-Institut für Kohlenforschung: Mülheim, Germany, 2011.

Conference Presentations

29. "Enabling Large-Scale Hybrid Density Functional Theory Based *Ab Initio* Molecular Dynamics in the Condensed Phase: Theory, Algorithm, and Performance", *Poster Presentation*, OpenEye Outstanding Junior Faculty Award in Computational Chemistry, American Chemical Society National Meeting: San Francisco, CA, 2020 (virtual).

28. "Attracting Opposites: Promiscuous Ion-π Binding in the Nucleobases", *Oral Communication*, 74$^{\text{th}}$ Northwest Regional Meeting of the American Chemical Society: Portland, OR, 2019.

27. "Attacking the Strong and Weak Scaling Limits in Linear Scaling Hybrid Density Functional Theory", *Oral Communication*, American Physical Society March Meeting: Boston, MA, 2019.

26. "The Dipole Polarizability of a Water Molecue in Liquid Water", *Oral Communication*, American Physical Society March Meeting: Baltimore, MD, 2016.

25. "Nuclear Quantum Effects in Liquid Water: A Highly Accurate Ab Initio Path-Integral Molecular Dynamics Study", *Oral Communication*, 248$^{\text{th}}$ American Chemical Society National Meeting: San Francisco, CA, 2014.

24. "Accurate and Efficient Treatment of Many-Body van der Waals Interactions: Theory and Applications", *Oral Communication*, 248$^{\text{th}}$ American Chemical Society National Meeting: San Francisco, CA, 2014.

23. "Nuclear Quantum Effects in Liquid Water: A Highly Accurate Ab Initio Path-Integral Molecular Dynamics Study", *Oral Communication*, American Physical Society March Meeting: Denver, CO, 2014.

22. "Many-Body van der Waals Interactions: Theory and Applications", *Oral Communication*, 245$^{\text{th}}$ American Chemical Society National Meeting: New Orleans, LA, 2013.

21. "Liquid Water from First Principles: The Importance of Exact Exchange, Dispersion Interactions, and Nuclear Quantum Effects", *Oral Communication*, 245$^{\text{th}}$ American Chemical Society National Meeting: New Orleans, LA, 2013.

20. "Liquid Water from First Principles: The Importance of Exact Exchange, Dispersion Interactions, and Nuclear Quantum Effects", *Oral Communication*, American Physical Society March Meeting: Baltimore, MD, 2013.

19. "Many-Body van der Waals Effects in Advanced Materials", *Oral Communication*, American Physical Society March Meeting: Baltimore, MD, 2013.

18. "The Effects of van der Waals Interactions on the Structure of Liquid Water", *Oral Communication*, 244$^{\text{th}}$ American Chemical Society National Meeting: Philadelphia, PA, 2012.

17. "Accurate and Efficient Treatment of Many-Body van der Waals Interactions with Applications in Biology, Chemistry, and Physics", *Oral Communication*, 244$^{\text{th}}$ American Chemical Society National Meeting: Philadelphia, PA, 2012.

16. "The Effects of van der Waals Interactions on the Structure of Liquid Water", *Oral Communication*, American Physical Society March Meeting: Boston, MA, 2012.

15. "An Efficient Real-Space Implementation of the van der Waals Energy and Analytical Forces in Plane-Wave Ab Initio Molecular Dynamics", *Oral Communication*, American Physical Society March Meeting: Dallas, TX, 2011.

14. "An Efficient Implementation of the Tkatchenko-Scheffler van der Waals Correction in Plane-Wave Ab Initio Molecular Dynamics: Application to Liquid Water Simulations", *Poster Presentation*, Ψ_k Conference: Berlin, Germany, 2010.

13. "Three-Body Corrections to Scaled Opposite Spin Second-Order Møller-Plesset Perturbation Theory", *Poster Presentation*, 2008 World Congress of the World Association of Theoretical and Computational Chemists (WATOC): Sydney, Australia, 2008.

12. "Efficient Resolution-of-the-Identity Implementation of Local Scaled Opposite Spin Second-Order Møller- Plesset Perturbation Theory: A Correlated Look at Mutual Orientation in the Fullerene Dimer", *Oral Communication*, 236$^{\text{th}}$ American Chemical Society National Meeting: Philadelphia, PA, 2008.

11. "Local and Canonical Resolution-of-the-Identity Second-Order Møller-Plesset Perturbation Theory with Application to the Dimers of Benzene and Fullerene", *Oral Communication*, 2008 Materials Research Society (MRS) Spring Meeting: San Francisco, CA, 2008.

10. "An Efficient Resolution-of-the-Identity Implementation of Local Scaled Opposite Spin Second-Order Møller- Plesset Perturbation Theory: A Correlated Look at Mutual Orientation in the Fullerene Dimer", *Poster Presentation*, Symposium in Honor of William A. Lester Jr.: Berkeley, CA, 2007.

9. "An Efficient Implementation of the Analytical Gradient of Dual-Basis Resolution-of-the-Identity Second-Order Møller-Plesset Perturbation Theory with Application to the Benzene Dimer", *Poster Presentation*, Molecular Quantum Mechanics (MQM) Meeting in Honor of Peter Pulay: Budapest, Hungary, 2007.

8. "Dual-Basis Methods for Electronic Structure Theory", *Poster Presentation*, Molecular Quantum Mechanics (MQM) Meeting in Honor of Peter Pulay: Budapest, Hungary, 2007.

7. "Local and Canonical Resolution-of-the-Identity Second-Order Møller-Plesset Perturbation Theory: Application to Alanine Tetrapeptide Conformational Energies", *Oral Communication*, 232$^{\text{nd}}$ American Chemical Society National Meeting: San Francisco, CA, 2006.

6. "Dual-Basis Methods for Electronic Structure Theory", *Poster Presentation*, 232nd American Chemical Society National Meeting: San Francisco, CA, 2006.

5. "A Resolution-of-the-Identity Implementation of the Local Triatomics-in-Molecules Model for Second-Order Møller- Plesset Perturbation Theory with Application to Alanine Tetrapeptide Conformational Energies", 2005 American Conference on Theoretical Chemistry (ACTC): Los Angeles, CA, 2005.

4. "Mechanisms of C-H Activation by Rhenium-Based Homogeneous Catalysis", *Poster Presentation*, Materials and Process Simulation Center 2004 Research Conference: Pasadena, CA, 2004.

3. "Electron Affinities, Singlet-Triplet Splittings, and Local Aromaticity Considerations in Pentalene Annulated Polycyclic Aromatic Hydrocarbons", *Oral Communication*, 61$^{\text{st}}$ Annual Meeting of the Oregon Academy of Science: McMinnville, OR, 2003.

2. "The Photoassisted Adsorption Enhancement of Tetrakis(4-carboxyphenyl)porphine onto Sintered Nanoparticulate Titanium Dioxide Electrodes", *Oral Communication*, 60$^{\text{th}}$ Annual Meeting of the Oregon Academy of Science: Forest Grove, OR, 2002.

1. "Artificial Photosynthesis: A Novel Approach to Solar Energy Conversion", *Poster Presentation*, Annual Meeting of the Society of Environmental Journalists: Portland, OR, 2001.

Research Grants and Funding

Alfred P. Sloan Foundation 2020–2022

Project Name:	*2020 Sloan Research Fellowship*
PIs:	**R. A. DiStasio Jr.**
Award:	$75,000
Award Number:	N/A
Award Period:	09/01/2020–08/31/2022
PI Effort:	N/A
PI Summer Salary:	N/A

National Science Foundation (NSF) 2020–2021

Center for Sustainable Polymers (CSP) Seed Research Grant

Project Name:	*Rational Design of High-Density Polyethylene with Targeted Physical Properties via Statistical Modeling of Molecular Weight Distributions*
PIs:	**R. A. DiStasio Jr.**
Award:	$70,000
Award Number:	N/A
Award Period:	08/01/2020–07/31/2021
PI Effort:	0.5 months
PI Summer Salary:	N/A

National Science Foundation (NSF) / Faculty Early Career Development Program 2020–2025

Project Name:	*CAREER: Accurate, Reliable, and Routine First-Principles Prediction of the Structure and Stability of Molecular Crystal Polymorphs*
PIs:	**R. A. DiStasio Jr.**
Award:	$650,000
Award Number:	CHE-1945676
Award Period:	03/01/2020–02/28/2025
PI Effort:	1.0 month
PI Summer Salary:	1.0 month

Department of Energy (DOE) / Energy Frontier Research Centers 2019–2020

EFRC: Center for Alkaline-Based Energy Solutions (CABES) Seed Research Grant

Project Name:	*Synthesis and Characterization of Mechanically and Chemically Robust Polynorbornenes For Anion Exchange Membranes*
PIs:	**G. W. Coates, R. A. DiStasio Jr., and Brett P. Fors**
Award:	$75,000 ($37,500 to R. A. DiStasio Jr.)
Award Number:	N/A
Award Period:	08/01/2019–07/13/2020
PI Effort:	TBD months
PI Summer Salary:	0.0 months

Jacobs Technion–Cornell Institute 2019–2020

Project Name:	*Julia and Joshua Ruch Exchange Program*
PIs:	**R. A. DiStasio Jr., A. Schmidt, and D. Zax**
Award:	$7,000 ($2,500 to R. A. DiStasio Jr.)
Award Number:	N/A
Award Period:	07/01/2019–06/30/2020
PI Effort:	N/A months
PI Summer Salary:	0.0 months

Semiconductor Research Corporation (SRC) 2019–2021

Project Name:	*Exploiting Competitive Interactions for Area-Selective Thermal and Plasma-Enhanced Thin Film Deposition*
PIs:	**R. A. DiStasio Jr. and J. R. Engstrom**
Award:	$300,000 ($120,000 to R. A. DiStasio Jr.)
Award Number:	2019-NM-2889
Award Period:	06/01/2019–05/31/2022
PI Effort:	0.5 months
PI Summer Salary:	0.0 months

Department of Energy (DOE) / Energy Frontier Research Centers 2018–2022

EFRC: Center for Alkaline-Based Energy Solutions (CABES)

Project Name:	*Center for Alkaline-Based Energy Solutions (CABES)*
PIs:	**H. D. Abruna, T. A. Arias, J. Brock, P. Chen, G. W. Coates, F. J. DiSalvo, R. A. DiStasio Jr., J. Feng, E. Giannelis, S. Hammes-Schiffer, L. Kourkoutis, T. Mallouk, M. Mavrikakis, D. A. Muller, K. Noonan, B. Pivovar, A. Singer, J. Suntivich, and P. Zelenay**
Award:	$10,750,000 ($400,000 to R. A. DiStasio Jr.)
Award Number:	DE-SC0019445
Award Period:	08/01/2018–07/31/2022
PI Effort:	0.5 months
PI Summer Salary:	0.5 months

National Science Foundation (NSF) / Materials Research Science and Engineering Centers 2017–2023

MRSEC: Cornell Center for Materials Research (CCMR)

Project Name:	*IRG: 2D Atomic Membranes for 3D Systems*
PIs:	**I. Cohen, E. Demaine, R. A. DiStasio Jr., P. McEuen, D. A. Muller, and J. Park**
Award:	$8,167,000 ($480,000 to R. A. DiStasio Jr.)
Award Number:	DMR-1719875
Award Period:	09/01/2017–08/31/2023
PI Effort:	0.5 months
PI Summer Salary:	0.0 months

Computer Allocations

Lawrence Berkeley National Laboratories / Department of Energy (DOE) 2020

National Energy Research Scientific Computing Center (NERSC)

Project Name:	*Simulating Hydroxide Diffusion in Anion Exchange Membranes*
PI:	**R. A. DiStasio Jr.**
Award:	9.0 M CPU Hours
Project Name:	*Benchmark Non-Equilibrium Potential Energy Surfaces for Covalent Interactions*
PI:	**R. A. DiStasio Jr.**
Award:	7.0 M CPU Hours
Project Name:	*Machine Learning to Reduce Basis Set Incompleteness Error in Quantum Chemical Calculations*
PI:	**R. A. DiStasio Jr.**
Award:	9.0 M CPU Hours
Project Name:	*Quantum Chemical Study of Area-Selective Atomic Layer Deposition*
PI:	**R. A. DiStasio Jr.**
Award:	9.0 M CPU Hours

Lawrence Berkeley National Laboratories / Department of Energy (DOE) 2019

National Energy Research Scientific Computing Center (NERSC)

Project Name: *Quantum Mechanical Design of Base-Stable Cationic Ionophores for Alkaline Fuel Cell Applications*
PI: **R. A. DiStasio Jr.**
Award: 6.8 M CPU Hours

Project Name: *Benchmark Non-Equilibrium Potential Energy Surfaces for Noncovalent Intermolecular Interactions*
PI: **R. A. DiStasio Jr.**
Award: 2.5 M CPU Hours

Project Name: *Quantum Chemical Study of Area-Selective Atomic Layer Deposition*
PI: **R. A. DiStasio Jr.**
Award: 3.5 M CPU Hours

Lawrence Berkeley National Laboratories / Department of Energy (DOE) 2018

National Energy Research Scientific Computing Center (NERSC)

Project Name: *Quantum Mechanical Design of Sustainable Aliphatic Polymers with High Glass-Transition Temperatures*
PI: **R. A. DiStasio Jr.**
Award: 12.75 M CPU Hours

Project Name: *Quantum Chemical Study of Area-Selective Atomic Layer Deposition*
PI: **R. A. DiStasio Jr.**
Award: 3.5 M CPU Hours

Project Name: *Potential Energy Surfaces of Ion-Pi Systems for Molecular Engineering Applications*
PI: **R. A. DiStasio Jr.**
Award: 2.25 M CPU Hours

Argonne National Laboratories / Department of Energy (DOE) 2018

ALCF Data Science Program (ADSP)

Project Name: *Constructing and Navigating Polymorphic Landscapes of Molecular Crystals (Renewal)*
PI: Alexandre Tkatchenko
Co-PIs: **R. A. DiStasio Jr.**, Marina Meila, Alvaro Vazquez-Mayagoitia
Award: 75 M CPU Hours

Lawrence Berkeley National Laboratories / Department of Energy (DOE) 2017

National Energy Research Scientific Computing Center (NERSC)

Project Name: *Polarizabilities and Dispersion Coefficients Across the Entire Range of Aqueous Molecular Geometries*
PI: **R. A. DiStasio Jr.**
Award: 1.0 M CPU Hours

Project Name: *Dipole Polarizability of a Condensed-Phase Water Molecule*
PI: **R. A. DiStasio Jr.**
Award: 1.0 M CPU Hours

Argonne National Laboratories / Department of Energy (DOE) 2017

ALCF Data Science Program (ADSP)

Project Name: *Constructing and Navigating Polymorphic Landscapes of Molecular Crystals*
PI: Alexandre Tkatchenko
Co-PIs: **R. A. DiStasio Jr.**, Marina Meila, Alvaro Vazquez-Mayagoitia
Award: 60 M CPU Hours

Argonne National Laboratories / Department of Energy (DOE) 2015

ASCR Leadership Computing Challenge (ALCC) Award

Project Name:	*Anomalous Density Properties and Ion Solvation in Liquid Water: A Path-Integral Ab Initio Study*
PI:	**R. A. DiStasio Jr.**
Co-PIs:	R. Car, M. Ceriotti, H-Y. Ko, F. Martelli, B. Santra, A. Selloni, and X. Wu
Award:	175 M CPU Hours

Argonne National Laboratories / Department of Energy (DOE) 2014

ASCR Leadership Computing Challenge (ALCC) Award

Project Name:	*Ion Solvation, Catalytic Interfaces, and Extreme Aqueous Environments: An Ab Initio Study of Liquid Water*
PI:	**R. A. DiStasio Jr.**
Co-PIs:	R. Car, M. Ceriotti, H-Y. Ko, D. Limmer, F. Martelli, B. Santra, and A. Selloni
Award:	350 M CPU Hours

Argonne National Laboratories / Department of Energy (DOE) 2013

ASCR Leadership Computing Challenge (ALCC) Award

Project Name:	*Ab Initio Quantum Liquid Water and Aqueous Ionic Solutions*
PI:	**R. A. DiStasio Jr.**
Co-PIs:	R. Car and B. Santra
Award:	250 M CPU Hours

Awards and Honors

OpenEye Outstanding Junior Faculty Award in Computational Chemistry, American Chemical Society 2020
Sloan Research Fellowship, Alfred P. Sloan Foundation 2020
CAREER Award, National Science Foundation 2020
Certificate of Mentorship, Research Experiences for Undergraduates, National Science Foundation 2019
Certificate of Mentorship, Cornell–Howard Hughes Medical Institute 2018
Certificate of Mentorship, Research Experiences for Undergraduates, National Science Foundation 2017
Certificate of Mentorship, Girls' Science, Technology, Engineering, and Mathematics 2014
Certificate of Mentorship, Research Experiences for Undergraduates, National Science Foundation 2013
Erwin Schrödinger Graduate Research Fellowship, University of Georgia, CCQC 2003
Outstanding Graduating Senior Award, Portland State University 2003
Undergraduate Teaching Assistant Award of Appreciation, Portland State University 2003
Undergraduate Research and Creative Activity Award, Portland State University 2002–2003
Clyde Johnson Award in Chemistry, Portland State University 2002–2003
Harold Zeh Scholarship, American Chemical Society (ACS) 2002–2003
Undergraduate Teaching Assistant Award of Appreciation, Portland State University 2002
Certificate of Appreciation for Mentors, Apprentices in Science and Engineering Program 2002
Certificate of Appreciation for Mentors, Siemens Westinghouse Science and Technology 2001
President's List, Portland State University (all terms in attendance) 2001–2003
Phi Kappa Phi, Portland State University 2000–2003
Golden Key National Honor Society, Portland State University 1999–2003
Dean's List, Portland State University (all terms in attendance) 1999–2003

Mentoring and Outreach

National Science Foundation 2019

Mentor for the Research Experiences for Undergraduates (REU) summer research program for undergraduate students.

Cornell–Howard Hughes Medical Institute 2018

Mentor for the Cornell-HHMI Accelerating Medical Progress through Scholarship (CHAMPS) program for undergraduate students.

National Science Foundation 2017

Mentor for the Research Experiences for Undergraduates (REU) summer research program for undergraduate students.

NYU Courant Institute of Mathematical Sciences 2014

Mentor for the Girls' Science, Technology, Engineering, and Mathematics (GSTEM) summer research program for female high school students.

National Science Foundation 2013

Mentor for the Research Experiences for Undergraduates (REU) summer research program for undergraduate students.

Saturday Academy 2002

Mentor for the Apprentices in Science and Engineering (ASE) summer research program for high school students.

Siemens Foundation 2001

Mentor for the Siemens Westinghouse Science and Technology (STEM) summer research program for high school students.

Professional Activities

Executive Committee

Cornell Center for Materials Research (CCMR) 2020–2022

Users' Advisory Council

Argonne National Laboratories and the U.S. Department of Energy (DOE) 2016–2017

Organization of Conferences and Workshops

American Physical Society (APS): Denver, CO 2020
Focus Session: *van der Waals Interactions in Molecules, Materials, and Complex Environments*

Northeast Regional Meeting (ACS-NERM): Binghamton, NY 2016
Focus Session: *Theoretical and Computational Chemistry*

Ψ_k Conference: San Sebastian-Donostia, Spain 2015
Symposium: *First-Principles Modeling of Non-Covalent Interactions*

Modeling Many-Body Interactions (MMBI15) Workshop: Lake Garda, Italy 2015
Symposium: *First-Principles Modeling of Non-Covalent Interactions*

American Physical Society (APS): Denver, CO 2014
Focus Session: *van der Waals Interactions in Complex Materials: Bridging Theory and Experiment*

Scientific Software Contributions

Quantum ESPRESSO 2009–present
Q-Chem 2004–present

Academic Journal/Proposal Peer Review

ACS Central Science, ACS Petroleum Research Fund, CECAM, Computer Physics Communications, Defense Threat Reduction Agency, International Journal of Quantum Chemistry, Journal of the American Chemical Society, Journal of Chemical Physics, Journal of Chemical Theory and Computation, Journal of Computational Chemistry, Journal of Physical Chemistry A, Journal of Physical Chemistry B, Journal of Physical Chemistry C, Journal of Physical Chemistry Letters, Journal of Physics: Condensed Matter, Macromolecules, Molecular Physics, National Science Foundation (NSF), Nature Chemistry, Nature Communications, Physical Chemistry Chemical Physics, Physical Review A, Physical Review B, Physical Review Letters, Proceedings of the National Academy of Sciences, Scientific Data, Scientific Reports, Science Advances, US Department of Energy (DOE) Office of Basic Energy Sciences, DOE Office of Science Graduate Student Research (SCGSR) Program, Defense Threat Reduction Agency, Argonne Leadership Computing Challenge (ALCC), Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Program

Professional Affiliations

American Physical Society (APS)	2005–present
American Chemical Society (ACS, Member No. 2299566)	2002–present
Society for Industrial and Applied Mathematics (SIAM)	2011–present

Postdoctoral Advisees at Cornell University

Dr. Hsin-Yu Ko	2019–present
Dr. Eric Fuemmeler (Staff Scientist, Mayo Clinic)	2018–2020
Dr. Ka Un Lao (Assistant Professor, Virginia Commonwealth University)	2016–2019
Dr. Kai Luo (Postdoctoral Researcher, University of Florida)	2015–2016
Dr. Rahul Maitra (Assistant Professor, India Institute of Technology Bombay)	2015–2016

Graduate Student Advisees at Cornell University

Brian Ernst	2016–present
Zachary Sparrow	2017–present
Yan Yang (MEng/MSE '16)	2016–present
Yang Yang	2016–present
Junteng Jia (MS/CCB '18, Staff Scientist, Google)	2015–2018
Lijie Tu (PhD/AEP '19, Staff Scientist, Facebook)	2016–2019
Chengyan Zhan (MS/CCB '18, Staff Scientist, Google)	2015–2018

Undergraduate Student Advisees at Cornell University

Dorothy Leung (CBE)	2019–present
Paul Joo (PHYS)	2017–present
Justin Lee (CBE)	2019–present
Richard Kang (CCB '19, PhD student, UC Berkeley)	2019–2020
Erdong Ding (visiting from Nankai University, PhD student, Rice)	2018–2019
Harmke van Dijk (PHYS)	2017–2019
Nikita Torosyan (CCB '18, PhD student, Yale)	2017–2018
Colin Gladue (CCB/MATH '16)	2016–2017
Jaclyn Lunger (MSE '17, PhD student, MIT)	2016–2017
Jonathan Wong (CCB '17, PhD student, UC Berkeley)	2016–2017
Tracy Doumit (CCB '17)	2015–2017
Peter Csernica (CCB '16, PhD student, Stanford)	2015–2016
Paul Varga (CBE '17, Automation and Control Specialists, LLC)	2015–2016
Kwang Woo (CCB '16, Peace Corps)	2015–2016

Interns and High School Student Advisees at Cornell University

Trine Quady (REU)	2020
Dzmitry Vaido (REU)	2019
Destiny Malloy (CHAMPS)	2018
Andrew Sullivan (Regis High School '18, Undergraduate Student, Columbia)	2017
Erika Tirado (REU)	2017

Professional Collaborators (Last 48 Months)

A. Ambrosetti (Padova), T. Arias (Cornell), A. Aspuru-Guzik (Harvard/Toronto), T. Bereau (Max Planck Institute for Polymer Research), N. Benedek (Cornell), B. Brooks (NIH), R. Car (Princeton), M. Ceriotti (EPFL), J. Chelikowsky (UT Austin), G. Coates (Cornell), I. Cohen (Cornell), A. Damle (Cornell), J. Engstrom (Cornell), B. Fors (Cornell), P. Giannozzi (Udine), S. Hammes-Schiffer (Yale), T. Hoye (Minnesota), M. Klein (Temple), L. Kronik (Weizmann), A. Levitt (INRIA), M. Mavrikakis, (Wisconsin, Madison), P. McEuen (Cornell), P. Milner (Cornell), D. Muller (Cornell), M. Neumann (Avantgarde Materials Simulation), S. Nazarenko (Southern Mississippi), J. Park (Chicago), M. Pavanello (Rutgers), A. Rappe (UPenn), A. Reilly (CCDC), M. Scheffler (FHI), A. Schmidt (Technion), A. Selloni (Princeton), Y. Shao (Oklahoma), M. Silberstein (Cornell), F. Stillinger (Princeton), A. Tkatchenko (Luxembourg), S. Torquato (Princeton), A. Vazquez-Mayagoitia (Argonne), O. A. von Lilienfeld (Basel), X. Wu (Temple), D. Zax (Cornell)