Devin Matthews, Ph.D.

Southern Methodist University
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Education

Postdoctoral Studies
Inst. for Comp. Eng. And Sciences, University of Texas at Austin, 2014-2018.

Ph.D. in Chemistry
Dept. of Chemistry, University of Texas at Austin, Aug. 2014.

B.S. in Chemistry with Honors
Dept. of Chemistry, University of Texas at Austin, May 2010.

Positions

2018-Present ***Southern Methodist University***, Assistant Professor of Chemistry

Awards and Honors

2015-2018	Arnold O. Beckman Postdoctoral Fellow.
2015	Frederick A. Howes Scholar in Computational Science award.
2013	1st place poster prize at the 7th Congress of Molecular Quantum Mechanics in Lugano, Switzerland.
2013	Research highlight in the 2013 issue of *DEIXIS*, the yearly DOE CSGF publication.
2010-2014	DOE Computational Science Graduate Fellow.
2008-2010	Beckman Scholar.

Professional Service

- Grant review panel for the DOE INCITE program (2018).
- Program committee for the 2018 Principles and Practice of Parallel Programming conference (a peer-reviewed research venue).
- 2017 and 2018 application screening committees for the DOE Computational Science Graduate Fellowship program.
- Mentored graduate students in both the Stanton and van de Geijn groups at UT Austin.
- Ad-hoc review for the NSF Software Infrastructure for Sustained Innovation (S2I2) program.
- Reviewer for papers submitted to the Journal of Physical Chemistry A, the Journal of Chemical Physics, the Journal of Chemical Theory and Computation, and other publications.

Teaching Experience

Molecular Sciences Software Institute, VA Tech

July 2017	Taught two-day lecture series on C++ programming, computer architecture, and high-performance computing in the context of quantum chemistry to a group of ~50 graduate students.

Dept. of Chemistry, UT Austin

Spring 2011	Teaching assistant for second semester physical chemistry laboratory with Dr. Robb Wilson. Responsibilities included running laboratory period and grading lab reports.
Fall 2009, Spring 2010	Teaching assistant for two semesters of introductory chemistry with Dr. David Laude. Responsibilities included leading a recitation period, holding regular office hours, and writing homework and test questions.

Presentations

D.A. Matthews, invited departmental seminar, Texas Christian University, Sep. 27, 2018.

D.A. Matthews, "Lots of Things Look Like Matrices" oral presentation given at the 6th BLIS Retreat in Austin, TX, Sep. 17-18 2018.

D.A. Matthews, "The Performance of CCSD(T)(a) for Core-Excitations and -Ionizations" poster given at the Beckman Scholars/A.O. Beckman Postdoc. Fellow/Beckman Young Investigator Symposium, Irvine, CA, Aug. 2018.

D.A. Matthews, invited departmental seminar, Southern Methodist University, Apr. 13 2018.

D.A. Matthews, "Revisiting the Direct Product Decomposition" oral presentation given at the 27th Austin Symposium on Molecular Structure and Dynamics at Dallas, TX, Mar. 3-5 2018.

D.A. Matthews, Henrik Koch, Sonia Coriani, "The Performance of CCSD(T)(a) for Core-Excitations and -Ionizations" poster presented at the 58th Sanibel Symposium in St. Simon's Island, GA, Feb. 18-23 2018.

D.A. Matthews, "High Performance and High Accuracy are Not Mutually Exclusive" plenary talk given at the 58th Sanibel Symposium in St. Simon's Island, GA, Feb. 18-23 2018.

D.A. Matthews, "I Don't Care About BLAS" oral presentation given at the 5th BLIS Retreat in Austin, TX, Sep. 18-19 2017.

D.A. Matthews, "High-Performance Tensor Contraction for Quantum Chemistry" oral presentation at the Simons Foundation Tensor Computation Workshop, Sep. 14-15 2017.

D.A. Matthews, "Efficient Implementations and Interfaces for Tensor Operations in Quantum Chemistry" poster given at the Beckman Scholars/A.O. Beckman Postdoc. Fellow/Beckman Young Investigator Symposium, Irvine, CA, Aug. 2017.

D.A. Matthews, "Simple spin-adaptation for equation-of-motion coupled-cluster theory" oral presentation given at the New Developments in Coupled-Cluster Theory workshop in Telluride, CO, July 31-Aug. 4 2017.

D.A. Matthews, “Tensors and the Power of Imagination” oral presentation given at the SIAM Conference on Computational Science and Engineering (CSE17) in Atlanta, GA, Feb. 27-Mar. 3 2017.

D.A. Matthews, “Aquarius and TBLIS: Orthogonal Axes in Multilinear Algebra (and some other directions too)” oral presentation given at the MolSSI Workshop on Core Software Blocks in Quantum Chemistry in Asilomar, CA, May 7-10 2017.

D.A. Matthews, “Keeping Quantum Chemistry Simple: Two Tales” poster given at the 57th Sanibel Symposium in St. Simon’s Island, GA, Feb. 19-24 2017.

D.A. Matthews, “Computer Science in Chemistry: from Matrices to Tensors and Beyond” invited graduate seminar, Texas A&M Dept. of Computer Science and Engineering, Nov. 28 2016.

D.A. Matthews, “Tensor Contraction without BLAS” poster at the 2016 International Conference for High Performance Computing, Networking, Storage and Analysis (SC16), Nov. 13-18 2016.

D.A. Matthews, “Tensor Contraction with BLIS” oral presentation given at the 4th BLIS Retreat in Austin, TX, Sep. 19-20 2016.

D.A. Matthews, “High-Performance Tensor Contraction without BLAS” poster given at the Beckman Scholars/A.O. Beckman Postdoc. Fellow/Beckman Young Investigator Symposium, Irvine, CA, Aug. 2016.

D.A. Matthews, “A ‘BLAS’ for tensors with portable high performance” oral presentation given at the 2016 Scientific Computing with Python (SciPy) conference in Austin, TX, July 11-17 2016.

D.A. Matthews, J.H. Baraban, J.F. Stanton, “A new ‘better than CCSD’ method for EOM-CC calculations” poster given at the 56th Sanibel Symposium in St. Simon’s Island, GA, Feb. 14-19 2016.

D.A. Matthews, “BLAS for Tensors: What, Why, and How” oral presentation given at the 3rd BLIS Retreat in Austin, TX, Sep. 28-29 2015.

D.A. Matthews, D. Batory, B. Marker, R.A. van de Geijn, “Opportunities in Computational Science to Advance Software Engineering” oral presentation given at the Computational Science & Engineering Software Sustainability and Productivity (CSESSP) Challenges workshop in Rockville, MD, Oct. 15-16 2015.

D.A. Matthews, "High-Performance Tensor Contraction without BLAS" poster given at the Beckman Scholars/A.O. Beckman Postdoc. Fellow/Beckman Young Investigator Symposium, Irvine, CA, Aug. 2015.

D.A. Matthews, L. Cheng, J.F. Stanton, "Accelerating the convergence of higher-order coupled cluster methods" oral presentation given at the New Developments in Coupled-Cluster Theory workshop in Telluride, CO, Aug. 3-7 2015.

D.A. Matthews, "Doing Computational Chemistry with Square Pegs and Round Holes" oral presentation at the 2015 DOE CSGF conference in Washington D.C., July 27-30 2015.

D.A. Matthews, F.G. Van Zee, J.F. Stanton, R.A. van de Geijn, "High-accuracy Quantum Chemistry on a Modern Linear Algebra Stack" poster given at the Software Infrastructure for Sustained Innovation (SI^2) Principal Investigator (PI) workshop in Arlington, VA, Feb. 17-18 2015.

D.A. Matthews, "Beyond GEMM: How Can We Make Quantum Chemistry Fast?" oral presentation given at the 2nd BLIS Retreat in Austin, TX, Sep. 25-26 2014.

D.A. Matthews, "AQUARIUS: Scalability and Extensibility by Design" oral presentation given at the 248th ACS National Meeting in San Francisco, CA, Aug. 10-14 2014.

D.A. Matthews and J.F. Stanton, "Non-orthogonal Spin-adaptation of Coupled Cluster Methods with Quadruple Excitations" oral presentation at the 2014 DOE CSGF conference in Washington D.C., July 14-17 2014.

D.A. Matthews, J.Z. Gong, and J.F. Stanton, "Automatic generation of analytic equations for vibrational and rovibrational constants from fourth-order vibrational perturbation theory" presentation at the 69th International Symposium on Molecular Spectroscopy in Champaign-Urbana, IL, June 16-20 2014.

D.A. Matthews, J.Z. Gong, and J.F. Stanton, "Rovibrational constants from fourth-order perturbation theory and the relationship to the contact transformation approach" oral presentation at the 69th International Symposium on Molecular Spectroscopy in Champaign-Urbana, IL, June 16-20 2014.

D.A. Matthews, "AQUARIUS: Scalability and Extensibility by Design" oral presentation and poster given at the USC High-Performance Tensor Software for Scientific Computing workshop in Laguna Beach, CA, Dec. 8-11 2013.

D.A. Matthews and J.F. Stanton, "When all you have is linear algebra, everything looks like a matrix" oral presentation given at the 1st BLIS Retreat in Austin, TX, Sep. 5-6 2013.

D.A. Matthews and J.F. Stanton, “NCC: A new, non-orthogonally spin-adapted CCSDTQ program for closed shell systems” poster given at the 7th Molecular Quantum Mechanics congress in Lugano, Switzerland, June 2-7 2013 and the 2013 DOE CSGF conference in Washington D.C., July 25-27 2013.

D.A. Matthews, J.Z. Gong, and J.F. Stanton, “Vibrational constants for triatomic molecules from fourth-order perturbation theory” oral presentation at the 68th International Symposium on Molecular Spectroscopy in Columbus, OH, June 17-21 2013.

D.A. Matthews, J.Z. Gong, and J.F. Stanton, “Rotational and rovibrational constants for triatomic molecules from fourth-order perturbation theory” oral presentation at the 68th International Symposium on Molecular Spectroscopy in Columbus, OH, June 17-21 2013.

D.A. Matthews and J.F. Stanton, “A Fully Spin-Adapted Approach to Closed-Shell CCSDTQ” poster given at the 14th International Congress of Quantum Chemistry in Boulder, CO, June 25-30 2012 and the 2012 DOE CSGF conference in Washington D.C., July 26-28 2012.

D.A. Matthews and J.F. Stanton, “Practical Limitations of the EOMDIP- and EOMDEA-CC Methods” poster given at the 14th International Congress of Quantum Chemistry in Boulder, CO, June 25-30 2012.

D.A. Matthews and J.F. Stanton, “An ab initio model Hamiltonian for the e'×e' and e'×e'' singlet states of Si_3” oral presentation at the 67th International Symposium on Molecular Spectroscopy in Columbus, OH, June 18-22 2012.

D.A. Matthews, “Arbitrary-order coupled cluster without Global Arrays” oral presentation given at the SIAM Parallel Processing meeting in Savannah, GA, Feb. 15-17 2012.

D.A. Matthews and J.F. Stanton, “Approaches to the Full CI Limit for Singlet Biradicals” poster given at the 2011 DOE CSGF conference in Washington D.C., July 21-23 2011.

D.A. Matthews and J.F. Stanton "An extension of the equation-of-motion coupled cluster method to biradicals with full and approximate triple excitations" poster given at the Beckman Scholars Symposium, Irvine, CA, July 2009.

D.A. Matthews and J.F. Stanton "Approaches to the full CI limit of $^1\Delta$ nitrene" poster given at the 13th International Congress of Quantum Chemistry in Helsinki, Finland, June 22-28 2009 and at the University of Texas College of Natural Sciences Undergraduate Research Fair, April 2009.

D.A. Matthews and J.F. Stanton "Quantitative analysis of Fermi resonances by harmonic derivatives of perturbation theory corrections" oral presentation at the ACS Regional Meeting in Little Rock, AK Oct. 1-4 2008.

D.A. Matthews, J. Vázquez and J.F. Stanton “A contact transformation approach to resonance in vibrational perturbation theory” poster given at the University of Texas College of Natural Sciences Undergraduate Research Fair, April 2008.

D.A. Matthews and J.F. Stanton "Theoretical studies of the fundamental and overtone spectrum of the water dimer” oral presentation at the 62nd International Symposium on Molecular Spectroscopy in Columbus, OH, June 18-22 2007.

Publications

D.A. Matthews, "On Extending and Optimizing the Direct Product Decomposition" *submitted to Mol. Phys.*

A. Tajti, J.F. Stanton, **D.A. Matthews**, P. Szalay, "Accuracy of coupled cluster excited state potential energy surfaces" *submitted to J. Chem. Theory Comput.*

P. Springer, **D.A. Matthews**, P. Bientinesi, "Spin summations: A high-performance perspective" *submitted to ACM Transactions on Mathematical Software*.

J.Z. Gong, **D.A. Matthews**, P.B. Changala, J.F. Stanton, "Fourth-order vibrational perturbation theory with the Watson Hamiltonian: Report of working equations and preliminary results" *J. Chem. Phys.* **149**, 114102, (2018).

W.J. Morgan, **D.A. Matthews**, M. Ringholm, J. Agarwal, J.Z. Gong, K. Ruud, W.D. Allen, J.F. Stanton, H.F. Schaefer III, "Geometric Energy Derivatives at the Complete Basis Set Limit: Application to the Equilibrium Structure and Molecular Force Field of Formaldehyde" *J. Chem. Theory Comput.* **14**, 1333 (2018).

J. Huang, **D.A. Matthews**, R.A. van de Geijn, "Strassen's algorithm for tensor contraction" *SIAM Journal on Scientific Computing* **40**, C305 (2018).

D.A. Matthews, "High-performance tensor contraction without Transposition" *SIAM Journal on Scientific Computing* **40**, C1 (2018).

J. Huang, L. Rice, **D.A. Matthews**, R.A. van de Geijn, "Generating families of practical fast matrix multiplication algorithms" in *2017 IEEE 31st International Symposium on Parallel Distributed Processing (IPDPS)* (2017), pp. 656-667.

J.J. Eriksen, K. Kristensen, **D.A. Matthews**, P. Jørgensen, J. Olsen, "Convergence of coupled cluster perturbation theory" *J. Chem. Phys.* **145,** 224104 (2016).

D.A. Matthews, J.F. Stanton, "A new approach to approximate equation-of-motion coupled cluster with triple excitations" *J. Chem. Phys.* **145**, 124102 (2016).

J.J. Eriksen, **D.A. Matthews**, P. Jørgensen, J. Gauss, "Assessment of the accuracy of coupled cluster perturbation theory for open-shell systems. II. Quadruples expansions" *J. Chem. Phys.* **144**, 194103 (2016).

J.J. Eriksen, **D.A. Matthews**, P. Jørgensen, J. Gauss, "Assessment of the accuracy of coupled cluster perturbation theory for open-shell systems. I. Triples expansions" *J. Chem. Phys.* **144**, 194102 (2016).

J.H. Baraban, **D.A. Matthews**, J.F. Stanton, "Communication: An accurate calculation of the S_1 C_2H_2 *cis-trans* isomerization barrier height" *J Chem. Phys.* **144**, 111102 (2016).

K. Kristensen, J.J. Eriksen, **D.A. Matthews**, J. Olsen, P. Jørgensen, "A view on coupled cluster perturbation theory using a bivariational Lagrangian formulation" *J. Chem. Phys.* **144**, 064103 (2016).

J. McClain, J. Lischner, T. Watson, **D.A. Matthews**, E. Ronca, S.G. Louie, T.C. Berkelbach, G. K.-L. Chan, "Spectral functions of the uniform electron gas via coupled-cluster theory and comparison to the GW and related approximations" *Phys. Rev. B* **93**, 235139 (2016).

D.A. Matthews, J.F. Stanton, "Accelerating the convergence of higher-order coupled cluster methods" *J. Chem. Phys.* **143**, 204103 (2015).

J.J. Eriksen, **D.A. Matthews**, P. Jørgensen, J. Gauss, "Communication: The performance of non-iterative coupled cluster quadruples models" *J. Chem. Phys.* **143**, 041101 (2015).

M.C. Thompson, J.H. Baraban, **D.A. Matthews**, J.F. Stanton, J.M. Weber, "Heavy atom vibrational modes and low-energy vibrational autodetachment in nitromethane anions" *J. Chem. Phys*. **142**, 234304 (2015).

T.L. Nguyen, H. Lee, **D.A. Matthews**, M.C. McCarthy, J.F. Stanton, "Stabilization of the simplest Criegee intermediate from the reaction between ozone and ethylene: A high-level quantum chemical and kinetic analysis of ozonolysis" *J. Phys. Chem. A* **119**, 5524 (2015).

D.A. Matthews, J.F. Stanton, "Non-orthogonal spin-adaptation of coupled cluster methods: A new implementation of methods including quadruple excitations" *J. Chem. Phys.* **142**, 064108 (2015).

J. Yang, W. Hu, D. Usvyat, **D.A. Matthews**, M. Schütz, G. K-L. Chan, "Ab initio determination of the crystalline benzene lattice energy to sub-kilojoule/mole accuracy" *Science* **345**, 640 (2014).

E. Solomonik, **D.A. Matthews**, J.R. Hammond, J.F. Stanton, J. Demmel, "A massively parallel tensor contraction framework for coupled-cluster computations" *J. Par. Dist. Comp.* **74**, 3176 (2014).

D.A. Matthews, J. Gauss, and J.F. Stanton, "Revisitation of non-orthogonal spin adaptation in coupled cluster theory" *J. Chem. Theory Comput.* **9**, 2567 (2013).

E. Solomonik, **D.A. Matthews**, J.R. Hammond, J.F Stanton, J. Demmel, “Cyclops tensor framework: Reducing communication and eliminating load imbalance in massively parallel contractions” in *2013 IEEE 27th International Symposium on Parallel Distributed Processing (IPDPS)* (2013), pp. 813–824.

D.A. Matthews, J.F. Stanton, "Quantitative analysis of Fermi resonances by harmonic derivatives of perturbation theory corrections" *Mol. Phys.* **107**, 213 (2009).

J.F. Stanton, B.A. Flowers, **D.A. Matthews**, A.F. Ware, G.B. Ellison, "Gas-phase infrared spectrum of methyl nitrate" *J. Mol. Spect.* **251**, 384 (2008).

H.G. Kjaergaard, A.L. Garden, G.M. Chaban, R.B. Gerber, **D.A. Matthews**, J.F. Stanton, "Calculation of vibrational transition frequencies and intensities in water dimer: comparison of different vibrational approaches" *J. Phys. Chem. A* **112**, 4324 (2008).

D.A. Matthews, J. Vázquez, J.F. Stanton, "Calculated stretching overtone levels and Darling-Dennison resonances in water: a triumph of simple theoretical approaches" *Mol. Phys.* **105**, 2659 (2007).