A. Eugene DePrince, III

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Education and Professional Experience

Florida State University	Associate Professor, 2018-present Department of Chemistry and Biochemistry
Florida State University	Assistant Professor, 2013-2018 Department of Chemistry and Biochemistry
Georgia Institute of Technology	Postdoctoral Fellow, 2011-2013 School of Chemistry and Biochemistry Advisor: Professor C. David Sherrill
Argonne National Laboratory	Postdoctoral Fellow, 2010-2011 Center for Nanoscale Materials Advisor: Dr. Stephen K. Gray
University of Chicago	Ph.D. in Chemistry, 2009 *A parametric approach to variational two-electron reduced-density-matrix theory.* Advisor: Professor David A. Mazziotti
University of Chicago	M.S. in Chemistry, 2006 Advisor: Professor David A. Mazziotti
University of Tennessee	B.S. in Chemistry, *summa cum laude*, 2005

Honors & Awards

ACS OpenEye Outstanding Junior Faculty Award	American Chemical Society COMP Division (2017)
Emerging Young Investigator	Florida Local Section of the ACS (2017)
Faculty Early Career Development (CAREER)	National Science Foundation (2016)
Ralph E. Powe Junior Faculty Enhancement Award	Oak Ridge Associated Universities (2015)
American Competitiveness in Chemistry Postdoctoral Fellowship	National Science Foundation (2011-2013)
Computational Postdoctoral Fellowship	Argonne National Laboratory, Division of Computing, Environment, and Life Sciences (2010-2011)
National Defense Science and Engineering Graduate Research Fellowship	Department of Defense (2005-2008)
Freud Scholar Fellowship	University of Chicago (2005)

Teaching

Florida State University

Instructor, CHM 5908: Focus on Physical Chemistry: Modern Electronic Structure Theory	S17
Instructor, CHM 4411: Physical Chemistry II	S18, S16, S15
Instructor, CHM 1050: Honors General Chemistry I	F15
Instructor, CHM 5480: Graduate Quantum Mechanics	F18, F16, F14
Instructor, CHM 5710: Chemical Structure and Bonding	F13
Supervisor, CHM 1051L: Honors General Chemistry II Research Laboratory	S16, S14
Supervisor, Directed Individual Study (five undergraduate students)	S18, F17, Su17, S17, F16, Su16, S16, F15, S14

Publications

Refereed Publications

(37) M. Mostafanejad and A. E. DePrince III, J. Chem. Theory Comput. **15**, 290-302 (2019). "Combining pair-density functional theory and variational two-electron reduced-density matrix methods."

(36) J. W. Mullinax, E. Epifanovsky, G. Gidofalvi, and A. E. DePrince III, J. Chem. Theory Comput. **15**, 276-289 (2019). "Analytic energy gradients for variational two-electron reduced-density-matrix methods within the density fitting approximation."

(35) E. Maradzike and A. Eugene DePrince III, J. Chem. Phys. **149**, 234101 (2018). "Modeling core-level excitations with variationally optimized reduced-density matrices and the extended random phase approximation."

(34) T. Banerjee, S. P. Hill, M. Hermosilla-Palacios, B. D. Piercy, J. Haney, B. Casale, A. E. DePrince III, M. D. Losego, V. D. Kleiman, and K. Hanson, J. Phys. Chem. C, **122**, 28478-28490 (2018). "Diphenylisobenzofuran bound to nanocrystalline metal oxides: excimer formation, singlet fission, electron injection, and low energy sensitization."

(33) N. Eldabagh, M. Micek, A. E. DePrince III, and J. J. Foley IV, J. Phys. Chem. C **122**, 18256-18265 (2018). "Resonance energy transfer mediated by metal-dielectric composite nanostructures."

(32) D. G. A. Smith, L. A. Burns, D. A. Sirianni, D. R. Nascimento, A. Kumar, A. M. James, J. B. Schriber, T. Zhang, B. Zhang, A. S. Abbot, E. Berquist, M. H. Lechner, L. dos Anjos Cunha, A. Heide, R. A. King, A. C. Simmonett, J. M. Turney, H. F. Schaefer, F. A. Evangelista, A. E. DePrince III, T. D. Crawford, K. Patkowski, and C. D. Sherrill, J. Chem. Theory Comput. **14**, 3504-3511 (2018). "Psi4NumPy: An interactive quantum chemistry programming environment for reference implementations and rapid development."

(31) D. R. Nascimento and A. E. DePrince III, J. Chem. Theory Comput. **14**, 2418-2426 (2018). "Spatial and spin symmetry breaking in semidefinite-programming-based Hartree-Fock theory."

(30) E. Maradzike, G. Gidofalvi, J. M. Turney, H. F. Schaefer III, and A. E. DePrince III, J. Chem. Theory Comput. **19**, 4113-4122 (2017). "Analytical energy gradients in variational two-electron reduced-density-matrix-driven complete active space self-consistent field methods."

(29) D. R. Nascimento and A. E. DePrince III, J. Phys. Chem. Lett. **8**, 2951-2957 (2017). "Simulation of near-edge X-ray absorption fine structure with time-dependent equation-of-motion coupled-cluster theory."

(28) R. M. Parrish, L. A. Burns, D. G. A. Smith, A. C. Simmonett, A. E. DePrince III, E. G. Hohenstein, U. Bozkaya, A. Y. Sokolov, R. Di Remigio, R. M. Richard, J. F. Gonthier, H. R. McAlexander, M. Saitow, X. Wang, B. P. Pritchard, H. F. Schaefer III, R. A. King, E. F. Valeev, F. A. Evangelista, J. M. Turney, T. D. Crawford, and C. D. Sherrill, J. Chem. Theory Comput. **13**, 3185-3197 (2017). "Psi4 1.1: An open-source electronic structure program emphasizing automation, advanced libraries, and interoperability."

(27) D. R. Nascimento and A. E. DePrince III, J. Chem. Theory Comput. **12**, 5834-5840 (2016). "Linear absorption spectra from explicitly time-dependent equation-of-motion coupled-cluster theory." (ACS Editors' Choice, November 2016)

(26) A. E. DePrince III, J. Chem. Phys. **145**, 164109 (2016). "Variational optimization of the two-electron reduced-density matrix under pure-state N-representability conditions."

(25) J. Fosso-Tande, T.-S. Nguyen, G. Gidofalvi, and A. E. DePrince III, J. Chem. Theory Comput. **12**, 2260-2271 (2016). "Large-scale v2RDM-driven CASSCF methods."

(24) J. Fosso-Tande, D. R. Nascimento, and A. E. DePrince III, Mol. Phys. **114**, 423-430 (2016). "Accuracy of two-particle N-representability conditions for describing different spin states and the singlet-triplet gap in the linear acene series."

(23) D. R. Nascimento and A. E. DePrince III, J. Chem. Phys. **143**, 214104 (2015). "Modeling molecule-plasmon interactions using quantized radiation fields within time-dependent electronic structure theory"

(22) S. K. Cary, M. Vasiliu, R. E. Baumbach, J. T. Stritzinger, T. D. Green, K. Diefenbach, J. N. Cross, K. L. Knappenberger, G. Liu, M. A. Silver, A. E. DePrince III, M. J. Polinski, S. M. Van Cleve, J. H. House, N. Kikugawa, A. Gallagher, A. A. Arico, D. A. Dixon, and T. E. Albrecht-Schmitt, Nat. Commun. **6**, 6827 (2015). "Emergence of californium as the second transitional element in the actinide series"

(21) D. B. Jeffcoat and A. E. DePrince III, J. Chem. Phys. **141**, 214104 (2014). "N-representability-driven reconstruction of the two-electron reduced-density matrix for a real-time time-dependent electronic structure method."

(20) D. R. Nascimento and A. E. DePrince III, J. Chem. Theory Comput. **10**, 4324 (2014). "A parametrized coupled-pair functional for molecular interactions: PCPF-MI."

(19) M. R. Kennedy, A. L. Ringer, A. E. DePrince III, M. S. Marshall, R. Podeszwa, and C. D. Sherrill, J. Chem. Phys. **140**, 121104 (2014). "Communication: Resolving the three-body contribution to the lattice energy of crystalline benzene: Benchmark results from coupled-cluster theory."

(18) A. E. DePrince III, M. R. Kennedy, B. G. Sumpter, and C. D. Sherrill, Mol. Phys. **112**, 844-852 (2014). "Density-fitted singles and doubles coupled cluster on graphics processing units."

(17) A. E. DePrince III and C. D. Sherrill, J. Chem. Theory Comput. **9**, 2687-2696 (2013). "Accuracy and efficiency of coupled-cluster theory using density fitting / Cholesky decomposition, frozen natural orbitals, and a t_1-transformed Hamiltonian."

(16) A. Chen, R. L. Miller, A. E. DePrince III, A. Joshi-Imre, E. Shevchenko, L. E. Ocola, S. K. Gray, U. Welp, and V. K. Vlasko-Vlasov, Small **9**, 1939-1946 (2013). "Plasmonic amplifiers: engineering giant light enhancements by tuning resonances in multiscale plasmonic nanostructures"

(15) A. E. DePrince III and C. David Sherrill, J. Chem. Theory Comput. **9**, 293-299 (2013). "Accurate noncovalent interaction energies using truncated basis sets based on frozen natural orbitals"

(14) A. E. DePrince III and D. A. Mazziotti, Mol. Phys. **110**, 1917-1925 (2012). "Connection of an elementary class of parametric two-electron reduced-density-matrix methods to the coupled electron-pair approximation"

(13) A. E. DePrince III, M. Pelton, J. R. Guest, and S. K. Gray, Phys. Rev. Lett. **107**, 196806 (2011). "Emergence of excited-state plasmon modes in linear hydrogen chains from time-dependent quantum mechanical methods"

(12) A. Chen, A. E. DePrince III, A. Demortiere, A. Joshi-Imre, E. V. Shevchenko, S. K. Gray, U. Welp, and V. K. Vlasko-Vlasov, Small **7**, 2365-2371 (2011). "Self-assembled large Au nanoparticle arrays with regular hot spots for SERS"

(11) C. A. Schwerdtfeger, A. E. DePrince III, and D. A. Mazziotti, J. Chem. Phys. **134**, 174102 (2011). "Testing the parametric two-electron reduced-density-matrix method with improved functionals: Application to the conversion of hydrogen peroxide to oxywater"

(10) A. E. DePrince III and J. R. Hammond, J. Chem. Theory Comput. **7**, 1287-1295 (2011). "Coupled cluster theory on graphics processing units I: The coupled cluster doubles method"

(9) Y. Wang, A. E. DePrince III, S. K. Gray, X. M. Lin, and M. Pelton, J. Phys. Chem. Lett. **1**, 2692-2698 (2010). "Solvent-mediated end-to-end assembly of gold nanorods"

(8) A. E. DePrince III and D. A. Mazziotti, J. Chem. Phys. **133**, 034112 (2010). "Isomerization of nitrosomethane to formaldoxime: Energies, geometries, and frequencies from the parametric variational two-electron reduced-density-matrix method"

(7) A. E. DePrince and R. J. Hinde, Nanoscale Res. Lett. **5**, 592-596 (2010). "Accurate computation of electric field enhancement factors for metallic nanoparticles using the discrete dipole approximation"

(6) A. E. DePrince III and D. A. Mazziotti, J. Chem. Phys. **132**, 034110 (2010). "Exploiting the spatial locality of electron correlation within the parametric two-electron reduced-density-matrix method"

(5) A. E. DePrince III and D. A. Mazziotti, J. Chem. Phys. **130**, 164109 (2009). "Open-shell molecular electronic states from the parametric two-electron reduced-density-matrix method"

(4) A. E. DePrince III and D. A. Mazziotti, J. Phys. Chem. B **112**, 16158-16162 (2008). "Molecular geometries and harmonic frequencies from the parametric two-electron reduced density matrix method with application to the HCN-HNC isomerization"

(3) A. E. DePrince III, E. Kamarchik, and D. A. Mazziotti, J. Chem. Phys. **128**, 234103 (2008). "Parametric two-electron reduced-density-matrix method applied to computing molecular energies and properties at nonequilibrium geometries"

(2) A. E. DePrince III and D. A. Mazziotti, Phys. Rev. A **76**, 042501 (2007). "Parametric approach to variational two-electron reduced-density-matrix theory"

(1) A. E. DePrince III and D. A. Mazziotti, J. Chem. Phys. **127**, 104104 (2007). "Cumulant reconstruction of the three-electron reduced density matrix in the anti-Hermitian contracted Schrodinger equation"

Book Chapters

A. E. DePrince III, J. R. Hammond, and C. D. Sherrill in *Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics*, R. Walker and A. Goetz, Eds. (Wiley: New York, 2015, ISBN: 978-1118661789). "Iterative coupled-cluster methods on graphics processing units."

Other manuscripts

A. E. DePrince III and J. R. Hammond, 2011 Symposium on Application Accelerators in High-Performance Computing (SAAHPC), 131-140 (2011). "Quantum chemical many-body theory on heterogeneous nodes"

A. E. DePrince III, J. R. Hammond, and S. K. Gray, Proceedings of SciDAC 2011, Denver, CO, July 10-14, 2011 . "Many-body quantum chemistry on graphics processing units"

A. E. DePrince III and S. K. Gray, arXiv:1005.4634v1 "Theoretical study of the implications of causality when inferring metamaterial properties"

Professional Service

Workshops, Conferences, and Symposia

Symposium Organizer, 256^{th} American Chemical Society National Meeting and Exhibition — August 19-23, 2018
Structural Photonics

Symposium Organizer, 255^{th} American Chemical Society National Meeting and Exhibition — March 18-22, 2018
Quantum Mechanics

Symposium Organizer, 254^{th} American Chemical Society National Meeting and Exhibition — August 20-24, 2017
Quantum Mechanics

Workshop Organizer, 2017 ACS Florida Annual Meeting and Exhibition — May 4, 2017
"Interactive Quantum Chemistry: an Introduction to the Open-Source Psi Program"

Symposium Organizer, 253^{rd} American Chemical Society National Meeting and Exhibition — April 2-4, 2017
"Strong electron correlation and nonadiabatic dynamics"

Symposium Organizer, 253^{rd} American Chemical Society National Meeting and Exhibition — April 4-6, 2017
Quantum Mechanics

Session Co-Organizer, ACS Florida Annual Meeting and Exposition (FAME) — May 5-6, 2017
Computational Chemistry Symposium

Conference Organizer, 2016 Meeting of the Southeast Theoretical Chemistry Association (SETCA) — May 2016

Session Organizer, ACS Florida Annual Meeting and Exposition (FAME) — May 7-9, 2015
Computational Chemistry Symposium

Session Organizer, ACS Florida Annual Meeting and Exposition (FAME) — May 9-10, 2014
Physical Chemistry Symposium

Session Organizer, Southeast Regional Meeting of the ACS — November 2013
Computational Chemistry General Symposium

Department and University Committees

Member, High-performance Computing Advisory Panel, Florida State University — May 2014 - present

Member, Graduate Recruiting and Admission Committee, Florida State University — 2013-present

Member, Laboratory and Computer Facility Committee, Florida State University 2014-present

Peer Review

Chemical Physics Letters, International Journal of Quantum Chemistry, Computational and Theoretical Chemistry, Journal of Chemical Physics, Theoretical Chemistry Accounts, Journal of Computational Chemistry, Journal of Chemical Theory and Computations, Physical Chemistry Chemical Physics, Computer Physics Communications, Journal of Physical Chemistry A, Journal of Physical Chemistry Letters

Grant Review

Army Research Office Chemical Sciences Division, National Science Foundation Division of Chemistry (CTMC), American Chemical Society Petroleum Research Foundation, Department of Energy SCGSR Program

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Grants

Active

co-PI: National Science Foundation, Advanced Cyberinfrastructure Division (ACI-1663636)
"Collaborative Research: SI2-SSI: Sustainable Open-Source Quantum Dynamics and Spectroscopy Software: Chronus Quantum"
September 1, 2017 – August 31, 2021, $366,309 (for FSU location)

PI: National Science Foundation, Chemistry Division (CHE-1554354)
"CAREER: Quantum-mechanical methods for electronic excited states in complex systems"
May 1, 2016 – April 30, 2021, $473,445

PI: Army Research Office, Small Buisiness Technology Transfer Program Phase II (69478CHST2)
"Parallel Two-Electron Reduced Density Matrix Based Electronic Structure Software for Highly Correlated Molecules and Materials"
September 1, 2016 – August 31, 2018 (currently awaiting approval for no-cost extension), $408,304 (for FSU location)

co-PI: Department of Energy, Energy Frontier Research Center (DE-SC001656)
"Center for Actinide Science and Technology"
August 2016 – July 2020, $10,000,000 (total award; funds one postdoc for DePrince)

Past

PI: American Chemical Society Petroleum Research Foundation (54668-DNI6)
"Fundamental Investigations of Plasmons and Electron Dynamics in Petroleum-Derived Polycyclic Aromatic Hydrocarbons"
September 1, 2014 – August 31, 2017, $110,000.

PI: Army Research Office, Small Buisiness Technology Transfer Program Phase I (65925CHST1)
"Parallel Two-Electron Reduced Density Matrix Based Electronic Structure Software for Highly Correlated Molecules and Materials"
September 5, 2014 – March 4, 2015, $58,657.

PI: FSU CRC First Year Assistant Professor Program
"Computational Studies of Plasmons in Polycyclic Aromatic Hydrocarbons"
May 5, 2014 – August 8, 2014, $20,000.

co-PI: Invincea
"Polymer-Embedded Gamma-Ray Detectors"
April 2014 – August 2014, $95,664 (total award).
