A. Eugene DePrince, III

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Education and Professional Experience

Florida State University	Professor, 2022-present Department of Chemistry and Biochemistry
Google Quantum	Visiting Researcher, 2022-present
Florida State University	Associate Professor, 2018-2022 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

Developing Scholar Award	Florida State University (2019)
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)
First Year Assistant Professor Award	Florida State University (2014)
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	S23, S21, S18, S16, S15
Instructor, CHM 1050: Honors General Chemistry I	F15
Instructor, CHM 5480: Graduate Quantum Mechanics	F22, F21, F19, F18, F16, F14
Instructor, CHM 5481: Graduate Advanged Quantum Mechanics	S19
Instructor, CHM 5710: Chemical Structure and Bonding	F13
Supervisor, CHM 1051L: Honors General Chemistry II Research Laboratory	S16, S14
Supervisor, Directed Individual Study (10 undergraduate students)	F22, F21, F19, F18, S18, F17, Su17, S17, F16, Su16, S16, F15, S14

Publications

Refereed Publications

(72) T. Zhang, S. Banerjee, L. N. Koulias, E. F. Valeev, A. E. DePrince III, and X. Li, submitted. "Dirac-Coulomb-Breit molecular mean-field exact-two-component relativistic equation-of-motion coupled-cluster."

(71) D. W. Berry, N. C. Rubin, A. O. Elnabawy, G. Ahlers, A. E. DePrince III, J. Lee, C. Gogolin, and R. Babbush, submitted. "Quantum simulation of realistic materials in first quantization using non-local pseudopotentials."

(70) A. E. DePrince III, Wiley Interdiscip. Rev. Comput. Mol. Sci. **14**, e1702 (2024). "Variational determination of the two-electron reduced density matrix: A tutorial review."

(69) D. B. Williams-Young, S. H. Yuwono, A. E. DePrince III, and C. Yang, J. Chem. Theory Comput. **19**, 9177-9186 (2023). "Approximate exponential integrators for time-dependent equation-of-motion coupled-cluster theory."

(68) Paul A. Johnson and A. E. DePrince III, J. Chem. Theory Comput. **19**, 8129-8146 (2023). "Single reference treatment of strongly correlated H_4 and H_{10} isomers with Richardson-Gaudin states."

(67) J. J. Foley IV, J. F. McTague, and A. E. DePrince III, Chem. Phys. Rev. **4**, 041301 (2023). "*Ab initio* methods for polariton chemistry."

(66) S. H. Yuwono and A. E. DePrince III, J. Chem. Phys. **159**, 054113 (2023). "N-representability violations in truncated equation-of-motion coupled-cluster methods."

(65) S. H. Yuwono, B. C. Cooper, and A. E. DePrince III, J. Chem. Phys. **159**, 044113 (2023). "Time-dependent equation-of-motion coupled-cluster simulations with a defective Hamiltonian."

(64) G. M. Jones, R. R. Li, A. E. DePrince III, and K. D. Vogiatzis, J. Phys. Chem. Lett. **14**, 6377-6385 (2023). "Data-driven refinement of the electronic energy from two-electron reduced-density-matrix theory."

(63) M. D. Liebenthal, N. Vu, A. E. DePrince III, J. Phys. Chem. A **127**, 5264-5275 (2023). "Assessing effects the effects of orbital relaxation and the coherent-state transformation in in quantum electrodynamics density functional and coupled-cluster theories."

(62) N. C. Rubin, D. W. Berry, F. D. Malone, A. F. White, T. Khattar, A. E. DePrince III, S. Sicolo, M. Kühn, M. Kaicher, J. Lee, and R. Babbush, PRX Quantum **4**, 040303 (2023). "Fault-tolerant quantum simulation of materials using Bloch orbitals."

(61) F. Kuriakose, M. Commodore, C. Hu. C. J. Fabiano, D. Sen, R. R. Li, S. Bisht, O. Ungor, X. Lin, G. F. Strouse, A. E. DePrince III, R. A. Lazenby, F. Mentink-Vigier, M. Shatruk, and I. Alabugin, J. Am. Chem. Soc. **144**, 23448-23464 (2022). "Design and synthesis of Kekulé and non-Kekulé diradicaloids via radical peri-annulation strategy: the power of seven Clar's sextets"

(60) N. Vu, G. M. McLeod, K. Hanson, and A. E. DePrince III, J. Phys. Chem. A **126**, 9303-9312 (2022). "Enhanced diastereocontrol via strong light-matter interactions in an optical cavity"

(59) J. D. Mallory and A. E. DePrince III Phys. Rev. A, **106**, 053710 (2022). "Reduced-density-matrix-based ab initio cavity quantum electrodynamics"

(58) R. R. Li, N. C. Rubin, and A. E. DePrince III, J. Chem. Theory Comput., **18**, 5966-5977 (2022). "Challenges for variational reduced-density-matrix theory: Total angular momentum constraints"

(57) C. L. Cortes, A. E. DePrince III, and S. K. Gray, Phys. Rev. A, **106**, 042409 (2022). "Fast-forwarding quantum simulation with real-time quantum Krylov subspace algorithms"

(56) M. D. Liebenthal, N. Vu, and A. E. DePrince III, J. Chem. Phys. **156**, 054105 (2022). "Equation-of-motion cavity quantum electrodynamics coupled-cluster theory for electron attachment"

(55) R. R. Li, M. D. Liebenthal, and A. E. DePrince III, J. Chem. Phys. **155**, 174110 (2021). "Challenges for variational reduced-density-matrix theory with three-particle N-representability conditions."

(54) N. C. Rubin and A. E. DePrince III, Mol. Phys. **119**, e1954709 (2021). "$\mathtt{p}^\dagger\mathtt{q}$: A tool for prototyping many-body methods for quantum chemistry."

(53) E. Epifanivsky *et al.*, J. Chem. Phys. **155**, 084801 (2021). "Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package."

(52) B. C. Cooper, L. N. Koulias, D. R. Nascimento, X. Li, and A. E. DePrince III, J. Phys. Chem. A, **125** 5438-5447 (2021). https://doi.org/10.1021/acs.jpca.1c01102 "Short iterative Lanczos integration in time-dependent equation-of-motion coupled-cluster theory."

(51) A. E. DePrince III, J. Chem. Phys. **154**, 094112 (2021). "Cavity-modulated ionization potentials and electron affinities from quantum electrodynamics coupled-cluster theory."

(50) X. Li, N. Govind, C. Isborn, A. E. DePrince III, and K. Lopata, Chem. Rev. **120**, 9951-9993 (2020). "Real-time time-dependent electronic structure theory."

(49) E. Maradzike, M. Hapka, K. Pernal, and A. E. DePrince III, J. Chem. Theory Comput. **16**, 4351-4360 (2020). "Reduced density matrix driven CASSCF corrected for dynamic correlation from the adiabatic connection."

(48) N. Vu and A. E. DePrince III, J. Chem. Phys. **152**, 244103 (2020). "Size-extensive seniority-zero energy functionals derived from configuration interaction with double excitations."

(47) D. G. A. Smith, L. A. Burns, A. C. Simmonett, R. M. Parrish, M. C. Schieber, R. Galvelis, P. Kraus, H. Kruse, R. Di Remigio, A. Alenaizan, A. M. James, S. Lehtola, J. P. Misiewicz, M. Scheurer, R. A. Shaw, J. B. Schriber, Y. Xie, Z. L. Glick, D. A. Sirianni, J. S. O'Brien, J. M. Waldrop, A. Kumar, E. G. Hohenstein, B. P. Pritchard, B. R. Brooks, H. F. Schaefer III, A. Y. Sokolov, K. Patkowski, A. E. DePrince III, U. Bozkaya, R. A. King, R. A. Evangelista, J. M. Turney, T. D. Crawford, and C. D. Sherrill, J. Chem. Phys. **152**, 184108 (2020). "Psi4 1.4: Open-source software for high-throughput quantum chemistry."

(46) M. Mostafanejad, M. D. Liebenthal, and A. E. DePrince III, J. Chem. Theory Comput. **16**, 2274-2283 (2020). "Global hybrid multiconfiguration pair-density functional theory."

(45) D. B. Williams-Young, A. Petrone, S. Sun, T. F. Stetina, P. Lestrange, C. E. Hoyer, D. R. Nascimento, L. Koulias, A. Wildman, J. Kasper, J. J. Goings, F. Ding, A. E. DePrince III, E. F. Valeev, and X. Li, Wiley Interdiscip. Rev. Comput. Mol. Sci. **10**, e1436 (2020). "The Chronus Quantum (ChronusQ) software package."

(44) N. Vu, I. Mitxelena, and A. E. DePrince III, J. Chem. Phys. **151**, 244121 (2019). "An adiabatic connection for doubly-occupied configuration interaction wave functions."

(43) M. Mostafanejad, J. Haney, A. E. DePrince III, Phys. Chem. Chem. Phys., **21**, 26492-26501 (2019). "Kinetic-energy-based error quantification in Kohn-Sham density functional theory."

(42) D. R. Nascimento and A. E. DePrince III, J. Chem. Phys., **151**, 204107 (2019). "A general time-domain formulation of equation-of-motion coupled-cluster theory for linear spectroscopy."

(41) A. Dragulescu-Andrasi, A. Filatov, R. Oakley, X. Li, K. Lekin, A. Huq, C. Pak, S. Greer, J. McKay, M. Jo, J. Lengyel, I. Hung, E. Maradzike, A. E. DePrince III, S. Stoian, S. Hill, Y.-Y. Hu, and M. Shatruk, J. Am. Chem. Soc. **141**, 17989-17994 (2019). "Radical dimerization in plastic organic crystal leads to structural and magnetic bistability with wide thermal hysteresis."

(40) L. N. Koulias, D. B. Williams-Young, D. R. Nascimento, A. E. DePrince III, and X. Li, J. Chem. Theory Comput. **15**, 6617-6624 (2019). "Relativistic real-time time-dependent equation-of-motion coupled-cluster."

(39) J. W. Mullinax, L. Koulias, E. Maradzike, M. Mostafanejad, E. Epifanovsky, G. Gidofalvi, and A. E. DePrince III, J. Chem. Theory Comput. **15**, 6164-6178 (2019). "A heterogeneous CPU + GPU algorithm for variational two-electron reduced-density matrix driven complete active space self-consistent field theory."

(38) R. R. Li and A. E. DePrince III, Phys. Rev. A **100**, 032509 (2019). "The role of orbital angular momentum constraints in the variational optimization of the two-electron reduced-density matrix."

(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. **13**, 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"

Grants

Active

"Polaritonic Quantum Chemistry"
PI: A. E. DePrince
National Science Foundation (CHE-2100984)
June 1, 2021 – May 31, 2024
$444,721

"Relativistic Quantum Dynamics in the Non-equilibrium Regime"
PI: A. E. DePrince
co-PIs: X. Li (U Washington), E. Valeev (Virginia Tech), C. Yang (Lawrence Berkeley National Lab)
Department of Energy (DE-SC0022263)
August 15, 2021 – August 14, 2025
$4,400,000 (total award), $1,160,000 (for FSU location)

"Collaborative Research: Frameworks: Sustainable Open-Source Quantum Dynamics and Software: Chronus Quantum"
PI: X. Li (U Washington)
co-PIs: A. E. DePrince, S. Hammes-Schiffer (Yale), E. Valeev (Virginia Tech)
National Science Foundation
July 2022 – June 2027
$550,000 (for FSU location)

"ACS Bridge Site for Transitional Master's Program at Florida State University"
PI: M. Shatruk (FSU)
co-PI: A. E. DePrince
American Chemical Society
April 1, 2021 – April 14, 2024
$180,000

Past

"CAREER: Quantum-mechanical methods for electronic excited states in complex systems"
PI: A. E. DePrince
National Science Foundation (CHE-1554354)
May 1, 2016 – April 30, 2022
$473,445

"Parallel Two-Electron Reduced Density Matrix Based Electronic Structure Software for Highly Correlated Molecules and Materials"
PI: A. E. DePrince
co-PIs: G. Gidofalivi (Gonzaga), E. Epifanovsky (Q-Chem, Inc.)
Army Research Office, STTR Sequential Phase 2 (W911NF-19-C0048)
August 12, 2019 – August 11, 2022
$996,269 (total award), $453,607 (for FSU location)

"Collaborative Research: SI2-SSI: Sustainable Open-Source Quantum Dynamics and Spectroscopy Software: Chronus Quantum"
PI: X. Li (U Washington)
co-PIs: A. E. DePrince, A. McCoy (U Washington), E. Geva (U Michigan)
National Science Foundation (OAC-1663636)
September 1, 2017 – August 31, 2021
$366,309 (for FSU location)

"Parallel Two-Electron Reduced Density Matrix Based Electronic Structure Software for Highly Correlated Molecules and Materials"
PI: A. E. DePrince
co-PIs: G. Gidofalvi (Gonzaga), E. Epifanovsky (Q-Chem, Inc.)
Army Research Office, STTR Phase II (W911NF-16-C-0124)
September 1, 2016 – August 31, 2019
$408,304 (for FSU location)

"Center for Actinide Science and Technology"
PI: T. Albrecht-Schmitt (FSU)
co-PIs: A. E. DePrince, plus many more.
Department of Energy, Energy Frontier Research Center (DE-SC001656)
August 2016 – July 2020
$10,000,000 (total award; funded one postdoc for DePrince)

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

"Parallel Two-Electron Reduced Density Matrix Based Electronic Structure Software for Highly Correlated Molecules and Materials"
PI: A. E. DePrince
co-PI: Y. Shao (Q-Chem, Inc.)
Army Research Office, STTR Phase I (W911NF-14-P-0032)
September 5, 2014 – March 4, 2015
$58,657

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

"Polymer-Embedded Gamma-Ray Detectors"
PI: M. Shatruk (FSU)
co-PIs: J. B. Schlenoff (FSU), K. Hanson (FSU), A. E. DePrince
Invincea
April 2014 – August 2014
$95,664 (total award)

Professional Service

Workshops, Conferences, and Symposia

Symposium Co-organizer, 264^{th} American Chemical Society National Meeting and Exhibition — August 21-25, 2022
Quantum Mechanics

Symposium Co-organizer, 263^{rd} American Chemical Society National Meeting and Exhibition — March 20-24, 2022
Quantum Mechanics

Symposium Co-organizer, 262^{nd} American Chemical Society National Meeting and Exhibition — August 22-26, 2021
Quantum Mechanics

Symposium Co-organizer, 261^{st} American Chemical Society National Meeting and Exhibition — March 21-25, 2021
Quantum Mechanics

Symposium Co-organizer, 260^{th} American Chemical Society National Meeting and Exhibition — August 23-27, 2020
Quantum Mechanics

Symposium Co-organizer, 259^{th} American Chemical Society National Meeting and Exhibition — March 22-26, 2020 (canceled: Covid-19)
Quantum Mechanics

Symposium Co-organizer, 258^{th} American Chemical Society National Meeting and Exhibition — August 25-29, 2019
Quantum Mechanics

Symposium Co-organizer, 257^{th} American Chemical Society National Meeting and Exhibition Quantum Mechanics: Strong Correlation	March 31-April 4, 2019
Symposium Co-organizer, 257^{th} American Chemical Society National Meeting and Exhibition Quantum Mechanics	March 31-April 4, 2019
Symposium Organizer, 256^{th} American Chemical Society National Meeting and Exhibition Structural Photonics	August 19-23, 2018
Symposium Organizer, 255^{th} American Chemical Society National Meeting and Exhibition Quantum Mechanics	March 18-22, 2018
Symposium Organizer, 254^{th} American Chemical Society National Meeting and Exhibition Quantum Mechanics	August 20-24, 2017
Workshop Organizer, 2017 ACS Florida Annual Meeting and Exhibition "Interactive Quantum Chemistry: an Introduction to the Open-Source Psi Program"	May 4, 2017
Symposium Organizer, 253^{rd} American Chemical Society National Meeting and Exhibition "Strong electron correlation and nonadiabatic dynamics"	April 2-4, 2017
Symposium Organizer, 253^{rd} American Chemical Society National Meeting and Exhibition Quantum Mechanics	April 4-6, 2017
Session Co-Organizer, ACS Florida Annual Meeting and Exposition (FAME) Computational Chemistry Symposium	May 5-6, 2017
Conference Organizer, 2016 Meeting of the Southeast Theoretical Chemistry Association (SETCA)	May 2016
Session Organizer, ACS Florida Annual Meeting and Exposition (FAME) Computational Chemistry Symposium	May 7-9, 2015
Session Organizer, ACS Florida Annual Meeting and Exposition (FAME) Physical Chemistry Symposium	May 9-10, 2014
Session Organizer, Southeast Regional Meeting of the ACS Computational Chemistry General Symposium	November 2013

Department and University Committees

Chair, Promotion and Tenure Committee, Department of Chemistry and Biochemistry	2023
Member, Faculty Evaluation Committee, Department of Chemistry and Biochemistry	2023
Member, Graduate Recruiting and Admission Committee, Department of Chemistry and Biochemistry	2013-2017, 2022-present
Member, GRiPE, Department of Chemistry and Biochemistry	2019-2020
Member, Executive Committee, Department of Chemistry and Biochemistry	2018-2020
Member, Graduate Curiculum and Advancement Committee, Department of Chemistry and Biochemistry	2021-2022
Member, Faculty Additions Committee, Department of Chemistry and Biochemistry	2020-2022
Member, Ralph E. Powe Award Limited Submission Review Team, Florida State University	2020

Chair, Graduate Recruiting and Admission Committee, Department of Chemistry and Biochemistry	2017-2021
Member, High-performance Computing Advisory Panel, Florida State University	May 2014 - present
Member, Laboratory and Computer Facility Committee, Department of Chemistry and Biochemistry	2014-2016
External Boards and Committees	
Member, Center for Nanoscale Materials Proposal Evaluation Board, Argonne National Laboratory	2020-2022

Presentations

Departmental and Divisional Seminars

A. Eugene DePrince III, "*Ab initio* cavity quantum electrodynamics." University of California Santa Cruz, Department of Chemistry Seminar (March 13, 2023).

A. Eugene DePrince III, "*Ab initio* cavity quantum electrodynamics." University of Missouri, Department of Chemistry Colloquium (February 24, 2023).

A. Eugene DePrince III, "*Ab initio* cavity quantum electrodynamics." The Ohio State University, Department of Chemistry and Biochemistry, Physical Chemistry Division Seminar (October 17, 2022).

A. Eugene DePrince III, "*Ab initio* cavity quantum electrodynamics." University of Tennessee, Department of Chemistry, Theoretical Chemistry Division Seminar (April 29, 2022).

A. Eugene DePrince III, "The uncertainty principle." University of Tennessee, Department of Chemistry, Undergraduate Research Symposium Plenary Seminar (April 30, 2022).

A. Eugene DePrince III, "Who needs wave functions, anyway?" Johns Hopkins, Department of Chemistry Seminar (Zoom, December 8, 2020).

A. Eugene DePrince III, "Who needs wave functions, anyway?" Georgia Tech, School of Chemistry and Biochemistry, Physical Chemistry Division Seminar (Zoom, October 27, 2020).

A. Eugene DePrince III, "Who needs wave functions, anyway?" University of South Carolina, Department of Chemistry Physical Chemistry Division Seminar, Columbia, SC (March 26, 2018).

A. Eugene DePrince III, "Quantum chemistry without wave functions." University of Tennessee, Department of Chemistry Physical Chemistry Division Seminar, Knoxville, TN (November 6, 2017).

A. Eugene DePrince III, "Quantum chemistry without wave functions." Middle Tennessee State University, Department of Chemistry Seminar, Murfreesboro, TN (November 3, 2017).

A. Eugene DePrince III, "Quantum chemistry without wave functions." Georgia Institute of Technology, School of Chemistry and Biochemistry Physical Chemistry Division Seminar, Atlanta, GA (April 21, 2017).

A. Eugene DePrince III, "Quantum chemistry without wave functions." University of California at Berkeley, Department of Chemistry Special Seminar, Berkeley, CA (April 7, 2017).

A. Eugene DePrince III, "Quantum chemistry without wave functions." Auburn University, Department of Chemistry and Biochemistry Colloquium, Auburn, AL (March 9, 2017).

A. Eugene DePrince III, "Quantum chemistry without wave functions." University of North Texas, Department of Chemistry Seminar, Denton, TX (Febrary 3, 2017).

A. Eugene DePrince III, "Quantum chemistry without wave functions." Argonne National Laboratory, Mathematics and Computer Science Division Seminar, Argonne, IL (January 17, 2017).

A. Eugene DePrince III, "Quantum chemistry without wave functions." University of Louisville, Department of Chemistry Seminar (Brown and Williamson Distinguished Guest Speaker), Louisville, KY (January 13, 2017).

A. Eugene DePrince III, "Large-scale variational 2-RDM-driven CASSCF methods." University of Georgia, Physical Chemistry Seminar, Athens, GA (October 21, 2016).

A. Eugene DePrince III, "Quantum chemistry without wave functions." Florida State University, Department of Physics Colloquium, Tallahassee, FL (October 20, 2016).

A. Eugene DePrince III, "Semidefinite-programming-based electronic structure theory." Florida State University, Department of Scientific Computing Seminar, Tallahassee, FL (October 5, 2016).

A. Eugene DePrince III, "Modern quantum chemistry: theory, software, and applications," William Patterson University of New Jersey, Department of Chemistry Seminar, Wayne, NJ (October 29, 2015).

A. Eugene DePrince III, "Modern Quantum Chemistry," Florida Southern College Department of Chemistry Seminar, Lakeland, FL (March 2015).

A. Eugene DePrince III, "Exploring alternatives to coupled cluster theory," University of Florida Department of Chemistry, Physical Chemistry Seminar, Gainesville, FL (April 15, 2014).

A. Eugene DePrince III, "Enabling high-accuracy quantum chemistry on large molecules: GPUs, natural orbitals, and local correlation approximations," Florida State University Department of Chemistry Biochemistry Seminar, Tallahassee, FL (January 16, 2013).

A. Eugene DePrince III, "Enabling high-accuracy quantum chemistry on large molecules: GPUs, natural orbitals, and local correlation approximations," University of California, Merced Department of Chemistry Seminar, Merced, CA (December 12, 2012).

A. Eugene DePrince III, "Enabling high-accuracy quantum chemistry on large molecules: GPUs, natural orbitals, and local correlation approximations," Villanova University Department of Chemistry Seminar, Philadelphia, PA (December 4, 2012).

A. Eugene DePrince III, "Enabling high-accuracy quantum chemistry on large molecules: GPUs, natural orbitals, and local correlation approximations," Gonzaga University Department of Chemistry Seminar, Spokane, WA (March 30, 2012).

A. Eugene DePrince III, "Frontiers in quantum chemistry: Theories and algorithms," University of Illinois Department of Chemistry Seminar, Urbana, IL (April 4, 2011).

Invited Web Series Presentations

A. Eugene DePrince III, "Reduced-density-matrix-based methods in Q-Chem for strongly-correlated electrons" Q-Chem Webinar 57, (Virtual, September 30, 2021).

A. Eugene DePrince III, "Coupled-cluster methods for light–matter interactions" Theory and Simulation of Electronic and Optical Processes in Molecules and Materials, a web series organized by Prof. Christine Aikens (Zoom, Feburary 2, 2021).

Invited Conference and Workshop Presentations

A. Eugene DePrince III, "Quantum error mitigation via reduced density matrix purification." Virginia Tech Quantum Swiss Summer Workshop, Riva San Vitale, Switzerland (June 29, 2023).

A. Eugene DePrince III, "N-representability errors in truncated equation-of-motion coupled-cluster methods." 3^{rd} Quantum International Frontiers, Łódź, Poland (June 23, 2023).

A. Eugene DePrince III, "*Ab initio* cavity quantum electrodynamics." Florida Annual Meeting and Exhibition (FAME), Palm Harbor, FL (August 5, 2022).

A. Eugene DePrince III, "Reduced-density-matrix-based *ab initio* cavity quantum electrodynamics." 264^{th} American Chemical Society National Meeting and Exhibition, Chicago, IL (August 23, 2022).

A. Eugene DePrince III, "*Ab initio* cavity quantum electrodynamics." 10^{th} triennial Conference on Molecular Quantum Mechanics (MQM), Blacksburg, VA (June 29, 2022).

A. Eugene DePrince III, "Strong light-matter interactions and angular momentum states from v2RDM theory." International Conference on Reduced Density Matrix Theory for Quantum Many-Fermion Systems, San Sebastien, Spain (June 15, 2022).

A. Eugene DePrince III, "*Ab initio* cavity quantum electrodynamics." 61^{st} Sanibel Symposium, St. Simon's Island, GA (February 14, 2022).

A. Eugene DePrince III, "Reduced-density-matrix-based descriptions of nondynamic and dynamic electron correlation" Low-scaling and unconventional electronic structure techniques (LUEST), a Telluride conference (Zoom, June 1 – June 5, 2020).

A. Eugene DePrince III, "Time-dependent equation-of-motion coupled cluster for linear spectroscopy" Workshop on New Developments in Coupled-Cluster Theory, Telluride, CO (July 29 - August 2, 2019).

A. Eugene DePrince III, "Reduced-density-matrix based approaches to dynamical and nondynamical electron correlation" 102^{nd} Canadian Chemistry Conference and Exhibition, Quebec, Canada (May 30 – April 1, 2019).

A. Eugene DePrince III, "Reduced-density-matrix based approaches to dynamical and nondynamical electron correlation" 2019 Middle Atlantic Regional Meeting of the ACS, Baltimore, MD (May 30 – April 1, 2019).

A. Eugene DePrince III, "Dynamical correlation models for variational two-electron reduced-density matrix methods" 257^{th} American Chemical Society National Meeting and Exhibition, Orlando, FL (March 31, 2019).

A. Eugene DePrince III, "Reduced-density-matrix-based descriptions of dynamical and nondynamical electron correlation" Emerging Tools for Designing Practical Next Generation Catalysts, Texas A&M at Qatar, Doha, Qatar (March 11, 2019).

A. Eugene DePrince III, "Time-dependent electronic structure methods for plasmon-molecule interactions" 256^{th} American Chemical Society National Meeting and Exhibition, Boston, MA (August 22, 2018).

A. Eugene DePrince III, "Density functional theory and two-electron reduced-density matrix methods" 256^{th} American Chemical Society National Meeting and Exhibition, Boston, MA (August 21, 2018).

A. Eugene DePrince III, "Reduced-density-matrix-based descriptions of dynamical and nondynamical electron correlation" Gordon Research Conference on Computational Chemistry, West Dover, VT (July 24, 2018).

A. Eugene DePrince III, "Dynamical correlation models for variational two-electron reduced-density-matrix-based complete active space self-consistent field theory" 2018 Meeting of the Southeast Theoretical Chemistry Association, Baton Rouge, New Orleans (May 19, 2018).

A. Eugene DePrince III, "Time-dependent electronic structure methods for plasmon-molecule interactions" American Physical Society March Meeting 2018, Los Angeles, CA (March 5, 2018).

A. Eugene DePrince III, "Analytic energy gradients, excited states, and pure-state N-representability in variational 2-RDM driven CASSCF" International Workshop on 'New challenges in Reduced Density Matrix Functional Theory: Symmetries, time-evolution and entanglement,' Lausanne, Switzerland (September 29, 2017).

A. Eugene DePrince III, "Broadband absorption spectra from explicitly time-dependent equation-of-motion coupled-cluster theory" Workshop on Nanomaterials: Computation,Theory,and Experiment, Telluride, CO (July 11-15, 2017).

A. Eugene DePrince III, "Quantum chemistry without wave functions" 2017 Meeting of the Southeast Theoretical Chemistry Association, Oxford, MS (May 19, 2017).

A. Eugene DePrince III, "Quantum chemistry without wave functions" Florida Annual Meeting and Exhibition (FAME) Emerging Young Investigator Symposium, Palm Harbor, FL (May 5, 2017).

A. Eugene DePrince III, "Introduction to Quantum Chemistry" 253^{rd} American Chemical Society National Meeting and Exhibition, San Francisco, CA (April 2, 2017).

A. Eugene DePrince III, "Analytic gradients and excitation energies from v2RDM-driven CASSCF methods." Southeast Regional Meeting of the ACS (SERMACS), Columbia, SC (October 23-26, 2016).

A. Eugene DePrince III, "Large-scale v2RDM-driven CASSCF." EMN Meeting on Computation and Theory, Las Vegas, NV (October 10-14, 2016).

A. Eugene DePrince III, "A simple quantum-mechanical method to simulate plasmon/molecule interactions in the time domain." Workshop on Excited States: Electronic Structure and Dynamics, Telluride, CO (July 13-17, 2015).

A. Eugene DePrince III, "A simple quantum-mechanical method to simulate plasmon/molecule interactions in the time domain." 2015 Meeting of the Southeast Theoretical Chemistry Association (SETCA), Orlando, FL (May 14-16, 2015).

A. Eugene DePrince III, "Electronic excitation energies from a time-dependent two-electron reduced-density-matrix method." 55^{th} Sanibel Symposium, St. Simon's Island, GA (February 15, 2015).

A. Eugene DePrince III, "Modeling light-molecule interactions in the time domain." Southeast Ultrafast Conference (SEUFC 2015), Tallahassee, FL (January 16, 2015).

A. Eugene DePrince III, "Time-dependent density-matrix methods" Workshop on Excited States and Time-dependent Electronic Structure Theory, Telluride, CO (July 15-18, 2014).

A. Eugene DePrince III, "Extracting excited states from a real-time time-dependent variational 2-RDM theory" 2014 meeting of the Southeast Theoretical Chemistry Association (SETCA), Atlanta, GA (May 17, 2014).

A. Eugene DePrince III, "Extracting excited states from a real-time time-dependent variational 2-RDM theory" ACS Florida Annual Meeting and Exhibition (FAME), Palm Harbor, FL (May 9, 2014).

Contributed Conference Presentations (Oral)

A. Eugene DePrince III, "*Ab initio* cavity quantum electrodynamics." 2022 Meeting of the Southeastern Theoretical Chemistry Association (SETCA), Atlanta, GA (May 20, 2022).

A. Eugene DePrince III, "Quantum error mitigation via reduced density matrix purification." Symposium on Quantum Science and Engineering at Florida State University, Tallahassee, FL, (March 4, 2022).

A. Eugene DePrince III, "Dynamical correlation models for variational two-electron reduced-density-matrix-based complete active space self-consistent field theory" 255^{th} American Chemical Society National Meeting and Exhibition, New Orleans, LA (March 20, 2018).

A. Eugene DePrince III, "Variational optimization of the two-electron reduced-density matrix under pure-state N-representability conditions." 57^{th} Sanibel Symposium, St. Simon's Island, GA (February 22, 2017).

A. Eugene DePrince III, "Large-scale variational 2-RDM-driven CASSCF methods." Theory and Applications of Computational Chemistry 2016, Seattle, WA (August 30, 2016).

A. Eugene DePrince III, "Linear-response absorption spectra from explicitly time-dependent CC2." 252^{nd} American Chemical Society National Meeting and Exhibition, Philadelphia, PA (August 23, 2016).

A. Eugene DePrince III, "Large-scale variational 2-RDM-driven CASSCF methods." ACS Florida Annual Meeting and Exhibition (FAME), Palm Harbor, FL (May 7, 2016).

A. Eugene DePrince III, "Large-scale variational 2-RDM-driven CASSCF methods." Southeast Regional Meeting of the ACS (SERMACS), Memphis, TN (November 6, 2015).

A. Eugene DePrince III, "A simple quantum-mechanical method to model plasmon/molecule interactions in the time domain." ACS Florida Annual Meeting and Exhibition (FAME), Palm Harbor, FL (May 8, 2015).

A. Eugene DePrince III, "Simulating plasmon-molecule interactions in the time domain", 249^{th} National Meeting of the American Chemical Society, Denver, CO (March 22, 2015).

A. Eugene DePrince III, "N-representability-driven reconstruction of the two-electron reduced-density matrix for a real-time time-dependent electronic structure method", Southeast Regional Meeting of the ACS, Nashville, TN (October 16-19, 2014).

A. Eugene DePrince III, "Extracting excited states from a real-time time-dependent variational 2-RDM theory," 248^{th} National Meeting of the American Chemical Society, San Fransisco, CA (August 14, 2014).

A. Eugene DePrince III and C. David Sherrill, "Density-fitted singles and doubles coupled cluster theory on graphics processing units," Southeast Regional Meeting of the ACS, Atlanta, GA (November 15, 2013).

A. Eugene DePrince III and C. David Sherrill, "Density fitting and frozen natural approximations in coupled cluster theory," ACS Florida Annual Meeting and Exposition (FAME), Palm Harbor, FL (May 2013).

A. Eugene DePrince III and David A. Mazziotti, "Parametric approaches to variational two-electron reduced-density-matrix theory," 242^{nd} National Meeting of the American Chemical Society, Denver, CO (August 2011).

A. Eugene DePrince III and Jeff R. Hammond, "Coupled-cluster theory on graphics processing units," 242^{nd} National Meeting of the American Chemical Society, Denver, CO (August 2011).

A. Eugene DePrince III and Jeff R. Hammond, "Coupled-cluster theory on graphics processing units," 43^{rd} Midwestern Theoretical Chemistry Conference, University of Notre Dame, South Bend, IN (2011).

A. Eugene DePrince III and David A. Mazziotti, "Treating Large Molecular Systems with Parametric Variational 2-RDM Methods," 41^{st} Midwestern Theoretical Chemistry Conference, Southern Illinois University, Carbondale, IL (2009).

A. Eugene DePrince III and David A. Mazziotti, "Parametric Variational 2-RDM Method," 40^{th} Midwestern Theoretical Chemistry Conference, University of Michigan, Ann Arbor, MI (2008).