ELVIS MARADZIKE

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AREAS OF INTEREST

Mathematical models and optimization, materials modeling, high performance computing.

EDUCATION

Florida State University 2014-2019
Tallahassee, FL

· Ph.D. in Chemistry, expected summer 2019
· M.Sc. in Chemistry, May 2017

Amherst College 2006-2010
Amherst, MA

· B.A. (majors: Physics, French).

RESEARCH EXPERIENCE

Florida State University 2014-Present
Department of Chemistry and Biochemistry*, Graduate Researcher, supervised by Professor A. Eugene DePrince, III*

· Developed a method to compute the remaining dynamical correlation energy for references computed with the variational two-electron reduced density matrix complete active space self-consistent field (v2RDM-CASSCF) method.
· Developed a method for computing excited states for v2RDM-CASSCF references using Rowe's equation of motion and the extended random phase approximation.
· Developed analytic gradients for the v2RDM-CASSCF method.
· Modeled electron-dynamics in linear polyacenes by time-dependent configuration interaction.

University of Cape Town 2011-2011
Scientific Computing Research Unit*, Research Intern*

· Worked on a project implementing genetic algorithms to parameterize a force field for carbohydrates. Mostly learned molecular mechanics, using the CHARMM force field, and scripting in Python.

Amherst College 2009-2010
Department of Physics*, Undergraduate Research Assistant*

· Investigated resonant tunneling in the magnetization of Mn_{12}-t-Bu-Ac, a single molecule magnet.
· Designed and machined an all-new goniometer for the lab's cryogenic probe.

PUBLICATIONS

1. **E. Maradzike** and A. E. DePrince, III, "Modeling core-level excitations with variationally optimized reduced-density matrices and the extended random phase approximation", *Journal of Chemical Physics,* **149 (23)**, 2018.

2. **E. Maradzike**, G. Gidofalvi, J.M. Turney, H.F. Schaefer, and A.E. DePrince III, "Analytic Energy Gradients for Variational Two-Electron Reduced-Density-Matrix-Driven Complete Active Space Self-Consistent Field Theory", *Journal of Chemical Theory and Computation*, **13 (9)**, 2017.

SELECTED PRESENTATIONS

American Chemical Society Spring National Meeting and Expo April 2019
Division of Computers in Chemistry: Quantum Mechanics

· Oral presentation: "A dynamical correlation model for v2RDM-CASSCF"

59th Sanibel Symposium February 2019

· Poster presentation: "A dynamical correlation model for v2RDM-CASSCF"

Gordon Research Conference, Computational Chemistry July 2018

· Poster presentation: "Modeling core-level excitations with variationally optimized reduced-density matrices and the extended random phase approximation'

Southeastern Theoretical Chemistry Association Meeting May 2018

· Oral presentation: "Modeling core-level excitations with variationally optimized reduced-density matrices and the extended random phase approximation'

Florida ACS Meeting May 2017

· Oral presentation: "Analytic Gradients for v2RDM-CASSCF methods'

AWARDS

Florida State University 2019

· Jyotsna Dalal Graduate Student Award in Physical Chemistry.

Florida State University 2018

· Philip Schlenoff Graduate Student Travel Award.

Florida State University 2016

· 2nd Best Poster Award, South East Theoretical Chemistry Conference meeting.

Amherst College 2009

· Gregory S. Call Research Program award. Funded research over the summer of 2009.

TEACHING EXPERIENCE

Florida State University 2014-15, 2018-19
Physical and General Chemistry*, Teaching Assistant*

· Demonstrated proper experimental technique and guided students through experiments.
· Attended lectures, tutored students and graded assignments.

Falcon College 2012-2014
Mathematics*, Teacher*

· Achieved a 100% pass-rate for my Advanced level class in the year 2013.
· Helped revive a school sponsored night school program for adults looking to retake the national high school examinations.

Amherst College 2009-2010
Physics*, Teaching Assistant*

· Supervised the lab portion of a course in classical mechanics; tutored modern physics.