Amiel Stephen Paz

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Education

	New York University	09/2018 - 01/2023
	Ph.D. Chemistry	
	Advisor: William J. Glover	
	Stanford University	09/2014 - 06/2018
	B.S. Bioengineering	
	B.S. Chemistry	

Honors and Awards

	Stanford Postdoctoral Recruitment Initiative in Sciences and Medicine (PRISM)	September 2022
	Accepted into the 10th cohort of the Stanford PRISM program	
	Air Force Office of Scientific Research (AFOSR) Scholar	July 2022
	2022 American Conference on Theoretical Chemistry	
	Outstanding Lightning Talk Award	July 2020
	2020 Virtual Conference on Theoretical Chemistry ([my lightning talk](#))	

Fellowships and Grants

	[**PRISM Baker fellowship**](#)	January 2023
	50% of Stanford's postdoc minimum for 12 months	
	NYU GSAS Dean's Conference Fund Grant	July 2022
	Awarded for ACTC 2022	
	NYU GSAS Dean's Travel Grant	February 2020
	Cancelled due to COVID-19 pandemic	

Publications

1. **A. S. P. Paz** and W. J. Glover, "Efficient analytical gradients of property-based diabatic states: Geometry optimizations for localized holes", *under review* (2023)

2. A. Humeniuk, **A. S. P. Paz**, Y. Cao, and W. J. Glover, "Role of electronic polarization in the primary charge-transfer states of the purple bacteria reaction center: A polarizable QM/MM study with the integral-exact direct reaction field method", *under review* (2022)

3. X. Li, X. Jia, **A. S. P. Paz**, Y. Cao, and W. J. Glover, "Evidence for water antibonding orbital mixing in the hydrated electron from its oxygen 1s X-ray absorption spectrum", *J. Am. Chem. Soc.* **144**, 19668-19672 (2022)

4. M. Chaudhary, Y. Mao, M. Kondappan, **A. S. P. Paz**, V. Ivannikov, T. Byrnes "Stroboscopic quantum nondemolition measurements for enhanced entanglement generation between atomic ensembles", *Phys. Rev. A* **105**, 022443 (2022)

5. **A. S. P. Paz**, N. S. Baleeva, and W. J. Glover, "Active orbital preservation for multiconfigurational self-consistent field", *J. Chem. Phys.* **155**, 071103 (2021)

6. **A. S. P. Paz**, and W. J. Glover, "Diabatic Many-Body Expansion: Development and Application to Charge-Transfer Reactions", *J. Chem. Theory. Comput.* **17**, 1497 (2021)

7. S. Jain, Q. Zhu, **A. S. P. Paz** T. Schlick, "Identification of novel RNA design candidates by clustering the extended RNA-As-Graphs library", *Biochim. Biophys. Acta Gen. Subj.* 1864(6):129534 (2020)

8. W. J. Glover, **A. S. P. Paz**, W. Thongyod, C. Punwong, "Analytical Gradients and Derivative Couplings for Dynamically Weighted Complete Active Space Self-Consistent Field", *J. Chem. Phys.* **151**, 201101 (2019)

Contributed Presentations

1. <u>Amiel S. P. Paz</u> and William J. Glover, "Pushing the boundaries: QM/MM simulations of excited-state dynamics in the condensed phase", Quantum Multiscale, November 5, 2022

2. <u>Amiel S. P. Paz</u>, Zhuofan Shen and William J. Glover, "Pushing the boundaries: QM/MM simulations of excited-state dynamics in the condensed phase", ACS Fall 2022, August 24, 2022

3. <u>Amiel S. P. Paz</u>, "Maintaining model active spaces across molecules and environments with AOP-MCSCF", TCFMS Developer's meeting, July 29, 2022

4. <u>Amiel S. P. Paz</u> and William J. Glover, "Origins of the Ultrafast Excited-State Relaxation of the Hydrated Electron", ACTC 2022, July 26, 2022

5. <u>Amiel S. P. Paz</u> and William J. Glover, "Analytical gradients for property-based diabatic states: Theory and application to charge-transfer reactions in DNA", ACS Fall 2021, August 26, 2021

6. <u>Amiel S. P. Paz</u> and William J. Glover, "Active orbital preservation for multiconfigurational self-consistent field", ACS Fall 2021, August 23, 2021

7. <u>Amiel S. P. Paz</u> and William J. Glover, "Active orbital preservation for multiconfigurational self-consistent field", Quantum Dynamics and Spectroscopy of Functional Molecular Materials and Biological Photosystems, Les Houches, May 5, 2021

8. <u>Amiel S. P. Paz</u>, "Analytical Gradients for Boys Diabatization", TeraChem Developers Meeting, September 23, 2020

9. <u>Amiel S. P. Paz</u> and William J. Glover, "The Diabatic Many-Body Expansion: Development and Application to Charge-Transfer Reactions", Virtual Conference on Theoretical Chemistry, July 2020

10. <u>Amiel S. P. Paz</u> and William J. Glover, "On-the-fly Diagnosis of Active Space Orbital Discontinuities for Nonadiabatic *Ab initio* Molecular Dynamics", 2019 International Symposium on Quantum Effects in Chemistry and Biology, June 3, 2019

Software Development

- TeraChem

  - Derived and implemented gradients for state-averaged complete active space self-consistent field (SA-CASSCF) dipoles and SA-CASSCF Boys diabatic states (yet to be published)

  - Implemented gradients, and derived and implemented nonadiabatic couplings for the Quasiparticle Energies (QE) method (yet to be published)

  - Implemented the AOP-MCSCF method for CASSCF initial orbital guesses

- FMS

  - Modified FMS/AIMS to allow for propagation and spawning on quasidiabatic electronic states, where the diabats are determined on-the-fly

- PyFragger

  - Actively developing the Glover group's in-house fragmentation code that allows for multi-state fragmentation through the diabatic many-body expansion (D-MBE) and freely interfaces with any electronic structure code (closed source until the end of the author's Ph.D.)