JAMES MAZZUCA(PHYSICAL)

RESEARCH ADVISOR: DR. SOPHYA GARASHCHUK

SUMMER BEFORE FIRST YEAR
Copenhaver Fellow under Professor Vitaly Rassolov

SECOND YEAR
Poster presentation at the Second Annual EPSCoR Conference; Served as a judge at the USC Science and Engineering Fair (also 3rd and 5th year)

FIFTH YEAR
Received the Lipscomb Award for the poster/talk "Modeling enzymatic proton transfer with quantum trajectories" at the USC Graduate Symposium

AFTER GRADUATION

Accepted position as Assistant Professor with the Department of Chemistry at Alma College in Alma, MI.

FACTS:

FIRST YEAR

- Joined Prof. Sophya Garashchuk's research group
- Teaching assistant in physical chemistry lab (fall) and honors general chemistry lab (spring)
- Provided free tutoring to undergraduate physical chemistry students (all 5 years)
- Took five graduate-level classes: Quantum Chemistry, Spectroscopy and Molecular Structure, Biosynthesis of Macromolecules, Statistical Mechanics, Multiscale Modeling

SECOND YEAR

- Passed oral and written comprehensive research plan (fall): Trajectory study of quantum effects of nuclear motion in proton transfer reactions
- Passed oral and written original research proposal (spring): Modeling through-space electron transfer in aqueous solution with a time-dependent wavepacket approach
- Spent the summer at Oak Ridge National Lab for research collaboration

THIRD YEAR

- Took a graduate level math course: Computational Math II
- Presented a physical chemistry divisional seminar: Description of proton transfer in soybean lipoxygenase-1 employing approximate quantum trajectory dynamics
- Poster presentation at SETCA 2012
- Participated in the USC Chemistry Outreach program (also 4th year)
- Attended a winter workshop: Theory Winter School: Computational Approaches for Electronic/Magnetic Materials
- Attended a summer workshop: VSCE Programming Heterogeneous Parallel Computing Systems

FOURTH YEAR

- Presented at the organic chemistry summer seminar series: Description of proton transfer in soybean lipoxygenase-1 employing approximate quantum trajectory dynamics
- Awarded a travel grant to present a poster at the conference: Advances in Quantum Chemistry: Interfacing Electronic Structure with Dynamics
- Teaching assistant for undergraduate physical chemistry lecture and recitation (spring)
- Mentored a high school student through the SPRI program
- Contributed talk at SETCA 2013: Description of proton transfer in soybean lipoxygenase-1 employing approximate quantum trajectory dynamics

FIFTH YEAR

- Developed a new experiment which has been implemented in the undergraduate physical chemistry lab at USC
- Mentored an undergraduate student in the Magellan Scholar research program
- Contributed talk at the APS national conference: QTES-DFTB dynamics study on the effect of substrate motion on quantum proton transfer in soybean lipoxygenase-1
- Wrote and defended dissertation: Approximate Quantum Trajectory Method for Modeling Chemical Reaction Dynamics: Application to Enzymatic Proton Transfer

REPRESENTATIVE PUBLICATIONS

L. Wang, J. W. Mazzuca, S. Garashchuk, and J. Jakowski. The hybrid Quantum Trajectory/Electronic Structure DFTB-based approach to Molecular Dynamics. Paper presented at XSEDE14 Annual Conference, 2014.

J. Mazzuca, S. Garashchuk, and J. Jakowski. Description of proton transfer in soybean lipoxygenase-1 employing approximate quantum trajectory dynamics. *Chem. Phys. Lett.* 542:153-158, 2012.

S. Garashchuk, J. Mazzuca, and T. Vazhappilly. Efficient quantum trajectory representation of wavefunctions evolving in imaginary time. *J. Chem. Phys.* 135:034104, 2011.