RAYMOND R SADEGHI

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Department of Chemistry

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### **Education:**

Ph.D., Chemical Physics, the University of Colorado, Boulder 1994 M.S, Computer Science, the University of Colorado, Boulder 2003 B.S., Chemistry, the University of Texas, 1989

### **Research:**

- Simulation of Chemical Reactions using Time-dependent wave packet propagator using fast Fourier Transform (publications 1-5)
- Simulation of photodissociation Dynamics of  $CO_2$  in the upper atmosphere using electronic structure calculation and wave packet propagator simulators. The work involved collaborating with the experiments done at Brown University in Peter Weber's laboratories. (publication 6)
- Simulation of Reaction in the bulk using Monte Carlo simulation (publication 10)
- Simulation of Reactions using Electron-Nuclear Dynamics for reaction of electrons with gaseous oxygen, hydrogen (University of Florida).
- Developed a faster Data Base using Oracle 8i (Dell Inc., Austin, TX)
- Kinetic modeling of combustion of methane using Runge-Kutta and techniques in the field of non-linear dynamics. The experiments were done at Argonne National Laboratories where we obtained the necessary rate-constants required for the simulations.

# **Employment History:**

8/2021 to Present:	Associate Professor of	f Instruction Department of	Chemistry University of Texas

at San Antonio

8/2012- 8/2021 Senior Lecturer, Department of Chemistry University of Texas at

San Antonio

8/06 Visiting researcher, Department of Chemistry & Biochemistry,

Texas Tech University

12/06 Visiting Scientist, Department of Chemistry & Biochemistry,

University of Colorado

9/05 –08/2020 Senior Lecturer, The University of Texas at San Antonio

7/05 – 8/05 Research associate, Physical Organic Chemistry, Department of Chemistry

& Biochemistry, University of Colorado at Boulder

8/01- 5/05 Lecturer, University of Colorado, Department of Chemistry

1/99 - 1/01	Lecturer, The University of Texas at San Antonio, Department of Chemistry
1/01-8/01	Dell Inc., Data Base Analyst
5/95-1/99	Post-doctoral research, The University of Florida, Gainesville, FL
4/95 - 8/95	Visiting Scientist, Physikalisch-Chemisches Institute Universitat Heidelberg, Heidelberg, Germany
8/91 - 12/91	Visiting Scientist, Institute Theoretical Physics, Santa Barbara, CA
8/89 - 4/94	Teaching Assistant, University of Colorado, Boulder, Department of Chemistry.

# **Courses Taught:**

Academic Inquiry & Scholarship: AIS 1203

#### Chemistry:

Basic Chemistry, General Chemistry 1 and 2, Quantitative Topics (Advanced Calculus), Physical Chemistry 1 and 2, Graduate Quantum Chemistry, Chemical Kinetics and Dynamics, General Chemistry 2 Laboratory coordinator (Fall 2012 to present)

### Mathematics:

Calculus 1, 2, 3 (taught at UTSA Department of Mathematics from Summer of 2006 to Fall 2018)

### **Publications:**

- 1. "High Energy Transition State Resonances in the H+ H<sub>2</sub> Reaction"; Sadeghi, R.; Skodje, R. T.; J. Chem. Phys. 98, 9208 (1993).
- 2. "Spectral Quantization of High Energy Transition State Resonances in the H+ H<sub>2</sub> Reaction"; Sadeghi, R.; Skodje, R. T.; J. Chem. Phys. 99, 5126 (1993).
- 3. "Spectral Quantization of Transition State Dynamics for the Three Dimensional H+ H<sub>2</sub> Reaction"; Skodje, R. T.; Sadeghi, R.; Krause, J. L.; Koppel H.; J. Chem. Phys. 101, 1725 (1994).
- 4. "Barriers, Thresholds, and Resonances: Spectral Quantization of the Transition State for the Collinear D+ H<sub>2</sub> Reaction"; Sadeghi, R.; Skodje, R. T.; J. Chem. Phys. 101, 1725 (1995).
- 5. "Spectroscopy of Potential Barriers: An Analytic Line-Shape Formula for Broad Resonances"; Sadeghi, R.; Skodje, R. T.; Phys. Rev. A 52, 1996 (1995).
- 6. ``Control of Transition State Spectra: Enhancement of Diffuse Structure in the Photodissociation Spectrum of  $CO_2$ "; Sadeghi, R.; Skodje, R. T.; J. Chem. Phys. 105, 7504 (1996).
- 7. "Quantum Dynamics at the Transition State: Spectral Quantization and

- Spectral Control applied to the FH<sub>2</sub> Photodetachment Process"; Skodje, R. T.; Sadeghi, R.; and Krause, J. L.; J. Chem. Soc. Faraday Trans. 93, 765 (1997).
- 8. "Control of Transition State Spectra: A Variational Algorithm"; Skodje, R.T.; Sadeghi, R.; and Krause, J. L.; Chemical Physics 240 (1999).
- 9. `Structure and Dynamics of the S<sub>3</sub> State of CS<sub>2</sub>"; Sadeghi, R.; Krause, J. L.; Skodje, R. T.; J. Chem. Phys. 107, 6570 (1997).
- 10. "The Dynamics of Proton Transfer in a Water Chain"; Sadeghi, R.; Cheng, H-P.; J. Chem. Phys. 111, 2086 (2000).
- 11. Coherent State Dynamics of H<sup>+</sup> + HF reaction at E<sub>lab</sub>=30 eV", Maiti, B., Sadeghi, R. Morales, J., Chem. Phys. 340, 105 (2007).
- 12. "Dynamics for the Dynamic Frank Harris: Exploring  $H^+ + CF_4$  Reaction at  $E_{Lab} = 20$  and 30 eV", B. Maiti, P. M. McLaurin, R. Sadeghi, S. A. Perera and <u>J. A. Morales</u>, International Journal of Quantum Chemistry, **109**, 3026-3035 (2009).

## **Work in Progress:**

Time-dependent semiclassical approach to a highly activated complex molecule", Sadeghi, R., (in preparation)

## **Conferences Attended and Presentations**

- 2/95 Poster Presentation "Control of Reaction Dynamics", Sanibel Annual Symposium, St. Augustine, FL
- 6/95 Invited Speaker "Photodissociation Dynamics of CO<sub>2</sub>", The Southeastern Conference on Theoretical Chemistry, Florida State University, Tallahassee, FL
- 10/96 Speaker, Chemistry Colloquium "Transition State Spectroscopy", Quantum Theory Project, University of Florida, Gainesville, FL
- 8/97 Poster Presentation "Resonance in Chemical Reactions", The Conference in Theoretical Chemistry, Park City, Utah.
- 2/98 Poster Presentation, Annual Sanibel Symposium, St. Augustine, FL
- 5/98 Invited Speaker "Proton Transfer in water-wires", The Southeastern Conference on Theoretical Chemistry, Florida State University, Tallahassee, FL