RAYMOND R SADEGHI
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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 Instruction Department of Chemistry University of Texas at San Antonio
8/2023-Present	Adjunct Faculty Texas A&M University 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 I, II, and III UTSA Department of Mathematics from Summer of 2006 to Fall 2018

Publications:

1. ``High Energy Transition State Resonances in the H+ H_2 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_2 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_2 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_2 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_2 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_3 State of CS_2"; 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^+ + HF reaction at E_{lab}=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 J. A. Morales**,** *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_2", 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