



CHEMISTRY & BIOCHEMISTRY

# SEMINAR PROGRAM

DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY  
UNIVERSITY OF OKLAHOMA

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We Are Pleased to Announce A Seminar  
Presented By

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University of Nevada, Reno  
Department of Chemistry

Friday, September 9, 2022  
4:15 pm  
SLSRC 3410/3430

## Spin-Dependent Processes in Chemistry

Electron spin is central to many chemical processes, including photoinduced intersystem crossing transitions, thermally activated spin-forbidden reactions, and spin crossovers in transition metal complexes. These processes play important roles in light-harvesting materials, transition metal catalysis, and molecular magnets. Therefore, the ability to accurately model spin-dependent processes in complex molecular systems on different time scales is critical. In the first part of the talk, I will discuss a convoluted history of electron spin in physics and chemistry. In the second part, I will introduce the nonadiabatic statistical theory (NAST) and nonadiabatic molecular dynamics (NAMD) — two complimentary methods we use to model the kinetics and dynamics of spin-dependent processes involving transitions between electronic states of different spin multiplicities. Finally, I will highlight several recent applications of these methods. These will include the use of NAST to understand the kinetics of spin-forbidden reactions and intersystem crossing transitions in large molecular systems, and the application of NAMD to the complex excited state relaxation involving multiple intersystem crossing and internal conversion transitions in 2-cyclopentenone, a molecule of moderate size.

### Biography

Dr. Sergey Varganov is an associate professor of theoretical and computational chemistry and chemical physics at the University of Nevada, Reno. He obtained his Ph.D. with Prof. Mark Gordon at Iowa State University and was a postdoctoral researcher with Prof. Peter Gill at the Australian National University and Prof. Todd Martinez at Sandford University. His research interests include development of nonadiabatic kinetics and molecular dynamics to study spin-dependent processes in photochemistry, astrochemistry, and molecular magnets.