

# CHEMISTRY DEPARTMENT SEMINAR



## Making Sense of Charge Transport in $\pi$ -Conjugated Molecular Electronics with Help of Computational Simulations and Mathematical Models

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Host: Sally Pias, PhD

Friday, February 02, 2024  
2:00 pm MST  
Lopez 106

### Abstract

*Fields of organic electronics and photovoltaics offer the potential to create clean and low-cost electronic devices with customizable mechanical and optical properties. However, establishing a structured, well-defined set of principles for the rational design of such functional materials is still a challenge. This is partly due to an incomplete understanding of charge transport in extended  $\pi$ -conjugated systems with varied topologies. In my presentation, I will demonstrate using different poly-*p*-phenylene ion radicals how the multi-state parabolic model (MPM), developed and validated using experimental data and quantum chemistry calculations, sheds light on the charge transfer phenomena. This model is instrumental in guiding the design and synthesis of next-generation  $\pi$ -conjugated materials for photovoltaic applications such as molecular wires, switches, and field-effect transistors. Following this discussion, I will briefly cover research activities in my group in the areas of biochemical simulations and organometallic catalysis.*

### Bio

*Marat R. Talipov is an Associate Professor in the Department of Chemistry and Biochemistry at New Mexico State University, Las Cruces. He obtained his Ph.D. in Chemistry, specializing in Mathematical and Quantum Chemistry, from Bashkir State University, where he focused on the theoretical investigation of short-living molecules, nitroso oxides. Before joining New Mexico State University, Marat held a postdoctoral position at Marquette University and a researcher position at the Institute of Organic Chemistry in Ufa, Russia.*

