THE UNIVERSITY OF ARIZONA

Arizona State University

# MateriAlZ Seminar Series

## Machine learning for chemical properties & materials

## Friday, October 16 2020, 11 am MST


### Abstract

Computer simulation is foundational to modern theoretical chemistry and materials models. Traditional methods are based on classical physics or quantum mechanical (QM) methods. Classical techniques are computationally efficient but have questionable accuracy. QM based methods tend to be more accurate, however, their computational scaling is frequently prohibitively expensive to treat realistic systems. Machine learning-based (ML) QM property predictors are capable of fitting directly to QM data with low error while remaining computationally as fast as classical techniques. I will talk on developing and applying various models for QM property prediction, which are trained to large QM datasets then shown to generalize well outside of the training set. The targeted properties include ground state potential energy, non-equilibrium molecular dynamics and chemical reactions, excited states, atomic charge schemes, reduced Hamiltonians. Our results show the applicability of these accurate ML property predictors to systems many times larger than those in the training set with a several magnitude speedup over reference QM methods, an exciting prospect for computational sciences.



**Dr. Sergei Tretiak**

**Los Alamos National Laboratory (LANL)**


Sergei Tretiak is a deputy group leader in the Theoretical Division at LANL and a LANL Fellow. His research interests include development of electronic structure methods for molecular optical properties, nonlinear optical response of organic chromophores, non-adiabatic dynamics of electronically excited states, optical response of confined excitons in conjugated polymers, carbon nanotubes, semiconductor nanoparticles, mixed halide perovskites and molecular aggregates, the use of Machine Learning and Data Science toward modeling of materials.

**Zoom link: https://arizona.zoom.us/j/84414125444**