## Prof. Kyle C. Hartig

Accurate modeling of optical spectra with absolute radiometric intensities is essential for nuclear forensics and characterizing prompt optical signals from nuclear detonations. This requires precise knowledge of the individual transition probabilities, known as Einstein A coefficients, for each spectral line. However, obtaining these coefficients theoretically or experimentally is often impractical because of the complex electronic structures and vast number of transitions involved. In this study, we explored the use of machine learning to predict Einstein A coefficients for atomic transitions. We evaluated models such as neural networks, stacked ensembles, and decision trees and found that gradient boosting algorithms performed best, achieving 87% precision on transitions from 36 elements. We extended the knowledge of the model to heavier elements by training it using the experimentally reported transition probabilities for uranium. Following the expansion, the model was cross-validated using the experimental values of atomic transitions not reported in NIST for other heavy elements (Gd, Np, and Eu). Finally, we used the plutonium spectra previously gathered at the Savannah River National Laboratory to estimate the temperature of the plutonium plasma. This work represents the first publication of accurate transition probabilities for plutonium, filling a critical gap in the atomic data necessary for precise spectral modeling and characterization of nuclear forensics. Enhancing these transition probability predictions improves the accuracy of the modeling of the optical spectra, which is critical for interpreting prompt optical signals from nuclear detonations. This advancement enables more effective characterization and rapid analysis of such events, contributing to national security by aiding the detection and understanding of nuclear detonations and proliferation activities. Finally, the initial work will be presented using a similar architecture for the prediction of thermochemistry and fluid dynamics parameters of actinides necessary for improving nuclear detonation modeling for nuclear forensic applications, such as prompt characterization and fallout forecasting.