Predicting the Stability of Superheavy Elements and Isotopes Using Machine Learning

Background and Motivation: The periodic table, a foundational tool in the world of chemistry and nuclear physics, currently recognizes elements up to atomic number 118, known as Oganesson (Og). The discovery and characterization of superheavy elements have opened doors to understanding the nuances of atomic structures and the potential for novel properties. As the boundary of the periodic table is pushed further, there is a growing curiosity about the existence and stability of elements beyond 118. Machine learning, with its capability to analyze vast datasets and discern patterns, presents a promising avenue to address this challenge.

Objectives and Methods: The primary objective of this study was to employ machine learning techniques to predict the stability, as represented by half-life, of superheavy elements beyond the currently known elements. The methodology was comprehensive:

- Data Cleaning and Visualization: An initial exploration involved cleaning the dataset and visualizing known features to understand their correlation with half-life.
- Feature Engineering: The dataset was enriched by:
    - Extracting additional information from chemical properties like the Orbital Shell, the degree to which the last shell is filled, and the azimuthal quantum number.
    - Incorporating special features such as whether the proton number is even, if the neutron number is even, and the presence of "magic numbers" which are specific numbers of protons or neutrons in a nucleus that result in more stable isotopes and elements.
    - Introducing 'border elements', which represented theoretical isotopes positioned 1 or 2 protons away from recognized stable isotopes and were assigned a hypothetical half-life of zero. For instance, if an isotope with 1 proton and 7 neutrons was the last stable one, 'border elements' of 1 proton with 8 and 9 neutrons were added.
    - Transforming existing features using mathematical functions such as squaring and logarithmic transformations.
- Feature Selection: To maintain model simplicity and robustness, relevant features were selected based on evaluations using graphs, visualizations, and metrics like Partial Dependence, Correlation, Mutual Information, and Feature Importance.
- Model Selection: Multiple models were evaluated using metrics such as R^2, MSE, MAE, RMSE, MedAE, and Cross-Validation. A novel evaluation strategy was adopted, treating the data akin to a time series problem. For instance, training on the first 70% of elements and predicting the subsequent 10%. This strategy aims to ensure the model's capability to extrapolate and predict the stability of elements that lie beyond the current boundary. Models such as XGBRegressor, SVR, and Neural Network were then hyper-tuned and compared to identify the most optimal solution for predicting superheavy element stability.

Results:

Island of Stability Predictions: The machine learning model's prediction for the 'island of stability' was consistent with widely accepted theoretical conceptions, suggesting a range of 120-130 protons. Notably, the model predicted an exceptionally stable element with 120 protons and 195 neutrons, which could last for hours. This prediction offers an exciting avenue for experimentalists to explore the creation of this element, potentially leading to groundbreaking discoveries.

Implementation of Theoretical Models: Six theoretical nuclear models were incorporated into the study: the Independent Particle Model, Liquid Drop Model, Fermi Gas Model, Collective Model, Two-Center Shell Model, and No-Core Shell Model. Features specific to each model were ingeniously engineered and used to train the established 'best' model on a random 30% of the dataset. The goal was to assess which theoretical model best captured the essence of an element's half-life. In evaluating the performance across various theoretical models, several observations were made. The Independent Particle Model faced significant challenges when it came to predicting the heaviest 10% of elements, a region known as the 'peninsula of stability'. Conversely, the Collective Model grappled with its predictions concerning 'border elements.' Interestingly, the Fermi Gas Model predominantly struggled with northern border elements, while the No-Core Shell Model found the southern border elements more challenging. Notably, the Two-Center Shell Model excelled in handling elements with a neutron-to-proton ratio (N/Z) less than 1, whereas both the Collective and Independent models performed better for elements where the N/Z ratio was greater than 1. A unique challenge presented itself in a specific anomalous region, characterized by around 80 to 90 protons and roughly 126 neutrons. In this distinct region, devoid of stable elements, the Two-Center Shell Model and the Independent Particle Model stood out, hinting at their refined comprehension of nuclear intricacies.

Implications: The findings advocate for a more integrated approach in nuclear physics, merging computational techniques with traditional theoretical models. Future research directions include:

Future Research:

1. Delving deeper into understanding why certain theoretical models excel in specific regions.
2. Leveraging advanced computational tools to achieve more refined results.
3. Collaborating with nuclear physicists to review and validate the work.
4. Continual refinement of the model as more information about nuclear physics becomes available.
5. Extending the model to predict not just when elements will decay, but also the specific decay types. Decay types in nuclear physics refer to the processes by which an unstable atomic nucleus loses energy by emitting radiation. Predicting these decay types provides insights into the nature of the unstable nucleus and has various applications.