# Deciphering Glass Dissolution Rates: A Machine Learning Perspective for Prediction and Interpretation

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**Abstract**

Understanding the long-term chemical resistance of glass is vital for safely immobilizing nuclear waste. However, predicting the dissolution rate of glass, which depends on factors like composition, pH, and temperature, is complex due to their intricate and nonlinear relationship. To address this challenge, we curated a comprehensive dataset comprising around 2100 glass compositions along with corresponding pH and temperature values. Further, we employed various machine learning models, including Artificial Neural Network and Xg-Boost, to predict glass dissolution rates. Results show that the Xg-Boost model performs reasonably well, achieving a training score R2 value exceeding 0.9 and accurately predicting dissolution rates. Furthermore, we explored the dependency of dissolution rates on composition, pH, and temperature using a game theory-based SHAP approach. Additionally, we transformed the composition into different descriptors to develop a universal model capable of predicting dissolution rates for compositions not present in the training dataset. Our results demonstrate that descriptor-based models perform comparably well to composition-based models, suggesting their potential as a generalized prediction tool for dissolution rates. Finally, we derived the functional form of dissolution rates in terms of various descriptors through symbolic regression, enabling the calculation of dissolution rates for any oxide glass compositions. Overall, this study sheds light on glass dissolution rates and facilitates the discovery of novel glass compositions for effective nuclear waste management.

**Keywords:** Nuclear Waste, Machine Learning, Glass

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