

Predicting Nuclear Waste Immobilization Glasses Corrosion by Machine Learning

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For reasons of cost and convenience, nuclear waste is typically immobilized via vitrification. Nuclear waste immobilization glasses are then subsequently stored in geological repositories and are expected to remain durable for millions of years. However, our lack of understanding of the geochemical processes governing the long-term corrosion of nuclear waste glasses (e.g., dissolution kinetics in confined/unconfined condition, long-term surface passivation, risk of corrosion resumption due to zeolite crystallization, etc.) has raised some concerns regarding the safety of waste immobilization activities [1]. Here, we adopt machine learning to predict the corrosion kinetics of nuclear waste immobilization glasses over varying timescales [2–4]. We show that machine learning models offer accurate predictions, which exhibit an excellent match with available experimental data. We demonstrate that the developed machine learning models can be used to efficiently discover new glassy wasteforms formulations featuring enhanced chemical durability.

[1] Zhen-Wu, Prentice, Ryan, Ellison, Bauchy & Sant (2020), *npj Mater. Degrad.* **4**, 1–12. [2] Krishnan, Mangalathu, Smedskjaer, Tandia, Burton & Bauchy (2018) *J. Non-Cryst. Solids* **487**, 37–45. [3] Liu, Fu, Yang, Xu & Bauchy (2019) *J. Non-Cryst. Solids X* **4**, 100036. [4] Liu, Zhang, Krishnan, Smedskjaer, Ryan, Gin & Bauchy (2019) *npj Mater. Degrad.* **3**, 1–12.