Earth Science Informatics (2026) 19:30
https://doi.org/10.1007/s12145-026-02094-x

RESEARCH

A machine learning framework to lanthanide element distribution and predictability from the northwestern Iranian karst bauxite deposits

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Received: 31 May 2025 / Accepted: 21 February 2026

Abstract

This study applies Extreme Gradient Boosting (XGBoost) to examine how geological age clustering affects the predictability of light rare earth elements (LREEs: La–Sm) and heavy rare earth elements (HREEs: Eu–Lu) in the northwestern Iranian karst bauxites. Major oxides and weathering indices (CIA and CIW) were used as predictors, revealing contrasting behaviors between the Paleozoic and Mesozoic deposits. LREEs exhibited high accuracy in the Mesozoic deposits, whereas HREEs achieved the best predictability in the Paleozoic samples, reflecting distinct mineralogical controls. Variability in cerium, linked to paleoredox conditions, reduces LREEs model performance in the Paleozoic, while phosphate phases strongly influence HREEs enrichment. Feature importance consistently identifies P_2O_5 as the dominant predictor for both LREEs and HREEs across all deposits, highlighting the key role of phosphate minerals in lanthanide incorporation, whereas major oxides contribute less. CIA and CIW further enhance predictive accuracy, indicating that subtle variations in paleoweathering conditions affect lanthanide distribution and model performance. The LREEs and HREEs prediction models demonstrate promising potential, and further cross-validation across global karst bauxite deposits could improve understanding of the factors controlling REEs distribution, ultimately supporting more efficient and cost-effective exploration strategies for these critical metals.

Keywords Northwestern Iranian karst bauxite deposits · XGBoost · Cerium · P_2O_5 · LREEs and HREEs predictability

Introduction

Rare earth elements (REEs), spanning atomic numbers 57 to 71 from lanthanum to lutetium, constitute a group of metals with remarkably similar chemical and physical properties. REEs are classified as critical raw materials in the latest Study on Critical Raw Materials for the EU (Grohol and Veeh 2023) and as critical minerals in both the 2022 U.S. Geological Survey report and the China's 2023 Critical Minerals List (Li et al. 2023). These elements play an essential role in advanced technologies and/or materials, including metallurgical processes, permanent magnets for electric motors and generators, lighting phosphors, catalysts, batteries, fiber optics, optical amplifiers, lasers, glass, and ceramics. China overwhelmingly dominates global REEs production, supplying 85% of light REEs (LREEs: La–Sm) and 100% of heavy REEs (HREEs: Eu–Lu+Y) (Grohol and Veeh 2023). The global REEs market is experiencing rapid growth, with a market value reaching $7.29 billion in 2023 and a compound annual growth rate of 10.8%. Despite their

Communicated by Hassan Babaie

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Published online: 02 March 2026