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Deciphering Mantle Plume-Derived Melts via Unsupervised Machine Learning

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Mantle plume-derived melts serve as a critical window into the material composition of the lower mantle, particularly of the Large Low-Shear-Velocity Provinces (LLSVPs), which dominate the lowermost mantle. Ocean Island Basalts (OIBs) are the most representative surface expressions of these deep processes. Despite the rapid accumulation of geochemical data, conventional statistical approaches struggle to capture the high-dimensional, nonlinear structure inherent in plume-related geochemical variability. While artificial intelligence (AI) methods have been applied to characterize OIBs, its "black-box" nature often hinders physical interpretation. Here, we develop an unsupervised machine learning framework that integrates geochemical indicators sensitive to partial melting, fractional crystallization, and mantle source heterogeneity as input features.

Our model categorizes global OIBs into 17 distinct clusters, recovering traditional geochemical mantle end-members such as DMM, HIMU, EM1, EM2, and FOZO, thereby demonstrating consistency with established petrogenetic frameworks. Notably, OIB samples with high $^{3}He/^{4}He$ ratios—a widely accepted tracer of deep, less-degassed mantle reservoirs—are significantly concentrated within the FOZO-like clusters, providing independent validation of the model's ability to isolate deep-mantle signatures.

Spatial analysis further reveals that two moderately enriched clusters, together with the FOZO-like cluster, dominate the global OIB distribution, suggesting that lower-mantle plume sources share a common compositional backbone despite regional variability. A direct comparison of OIBs associated with the two major LLSVPs demonstrates remarkably similar clustering structures, implying that their material compositions are fundamentally comparable. However, systematic differences in enrichment levels occur both between and within the two LLSVP domains. This internal geochemical heterogeneity likely reflects the long-term impact of oceanic slab subduction and supercontinent cycles on the deep mantle, highlighting the dynamic coupling between surface tectonics and deep-mantle evolution.