Response to Reviewer #2

General Assessment:

The study addresses a significant knowledge gap in high-altitude, cold-arid ecosystems. The application of machine learning for spatial prediction is appropriate and modern. The manuscript is generally well-structured, but several aspects require clarification, strengthening, and more in-depth discussion before it can be considered for publication.

[Response] We appreciate the reviewer's positive comments and constructive suggestions on our manuscript, which have been carefully addressed in the revised version. We provide detailed point-by-point responses below, and we believe these revisions have substantially improved the quality and scientific rigor of the work.

Major Comments:

[Comment 1] There is a critical ambiguity regarding the analytical method for the core six micronutrients (Fe, Mn, Cu, Zn, Ni, Mo). The text states a portable XRF was used in the field (Lines 55-56) but later describes lab-based wavelength-dispersive XRF on pressed pellets (Lines 59-61). The accuracy and validation of field-based XRF measurements for these elements, especially at low concentrations (e.g., Mo), must be explicitly detailed. The authors should clarify the protocol, report calibration metrics (R^2, RMSE) against certified standards, and specify if all element data came from the same method.

[Response] Many thanks for raising this important concern. In our study, we initially used a second-generation portable XRF to conduct in situ measurements (n=130), but because this device could not reliably detect Mo, a key micronutrient of our focus, all samples were re-analyzed in the laboratory using a third-generation XRF with improved detection accuracy. **All data reported in this study for core micronutrients (Fe, Mn, Cu, Zn, Ni, Mo, V) were obtained from laboratory-based wavelength-dispersive XRF (third-generation XRF) on air-dried, and sieved (<2 mm) samples.**

To further validate the data quality, 218 randomly selected samples were re-analyzed using reviewer mentioned ICP-MS, a widely accepted traditional methods. Strong correlations were observed between XRF and ICP-MS for Fe, Mn, Cu, V (R^2 = 0.7-0.9; **Figure R1**), closely aligning with the 1:1 line. For Zn and Ni, significant correlations were also found (R^2 = 0.4-0.5), though with systematic deviations from the 1:1 line. Taking ICP-MS as the benchmark, XRF slightly over- or underestimated absolute contents. Importantly, these deviations do not substantially affect spatial distribution patterns central to this study for the following reasons: First, the XRF-based observed values are highly correlated with the XRF-based predicted values, and the ICP-MS-based observed values are also highly correlated with the ICP-MS-based predicted values (R^2 = 0.85-0.95; **Figure R2**). Second, we calibrated XRF-based Zn, and Ni using the regression relationships between the two methods and repeated spatial mapping. Results show that the spatial distribution patterns before and after calibration were highly consistent (R^2=0.8-0.9; **Figure R3**), confirming that the main conclusions are not sensitive to these measurement uncertainties. Third, for Mo, the results obtained from the two methods were not fully consistent, likely due to its low content. The XRF-based measurements may involve considerable uncertainties (**Figure R4**). Therefore, we have included both the observational and predicted results in the supplementary materials and discussed their potential uncertainties in detail in the Discussion section.

We have added data quality control details in the Methods section as follows: *"To ensure the reliability of soil micronutrient measurements, we adopted a two-step analytical strategy. First, in situ measurements were conducted using a second-generation portable Niton X-ray fluorescence (XRF) analyzer to obtain preliminary contents under natural field conditions. However, because this instrument could not reliably detect Mo, all soil samples were subsequently air-dried, sieved (2 mm), and re-analyzed in the laboratory using a third-generation XRF. Compared with the second-generation device, the third-generation XRF offers an extended detection range and improved accuracy (Lemière, 2018). All data presented in this study are based on the laboratory XRF measurements".*

To further validate the laboratory XRF results, a subset of 218 samples was randomly selected and re-analyzed using ICP-MS, a widely accepted reference method (Simon, 2005). The two methods showed strong correlations for Fe, Mn, V and Cu (R^2 = 0.67–0.89, $P<0.001$), with values closely aligning with the 1:1 line, indicating reliable quantification. For Zn and Ni, XRF and ICP-MS results were also significantly correlated, though systematic deviations from the 1:1 line were observed. XRF tended to slightly over- or underestimated absolute contents of Zn and Ni *contents compared with ICP-MS. To address this, we calibrated Zn and Ni, using the regression relationships between the two methods and then repeated spatial mapping. Comparative results of both methods are provided in the Supplementary Information*".

We discussed methodological uncertainties in the Discussion as follows: "*Although the laboratory XRF measurements used in this study were validated against ICP-MS and generally showed strong correlations, several limitations should be noted. For Fe, Mn, V and Cu, the two methods produced highly consistent results, supporting the robustness of the dataset. In contrast, Zn and Ni, exhibited systematic deviations from the 1:1 line, with XRF tending to slightly over- or underestimate contents relative to ICP-MS. These deviations likely arise from element-specific detection sensitivities of XRF. To address this, we calibrated Zn and Ni, using the regression relationships between the two methods and then repeated spatial mapping. The results before and after calibration were not significantly different, confirming that these deviations do not affect our main findings. Nonetheless, we acknowledge that incorporating ICP-based measurements on a larger sample set would further strengthen the accuracy of the dataset, and future efforts should consider combining multiple analytical approaches to minimize methodological uncertainties"*. For Mo, the results obtained from the two methods were not fully consistent, likely due to its low content. The XRF-based measurements may involve considerable uncertainties. Therefore, we have included both the observational and predicted results in the supplementary materials and discussed their potential uncertainties in detail in the Discussion section. Also, we added pixel-level uncertainty layers with the maps for users to properly utilize these datasets.

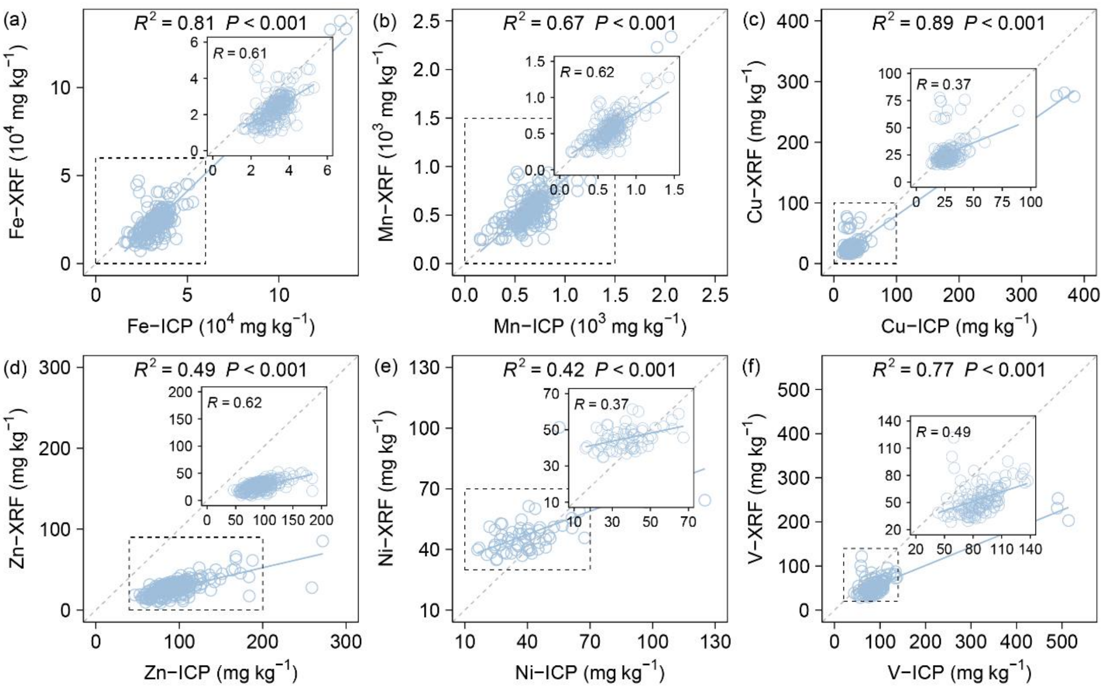

Figure R1. Comparison between laboratory-based third-generation XRF and ICP-MS measurements for six soil micronutrients (Fe, Mn, Cu, Zn, Ni, V).

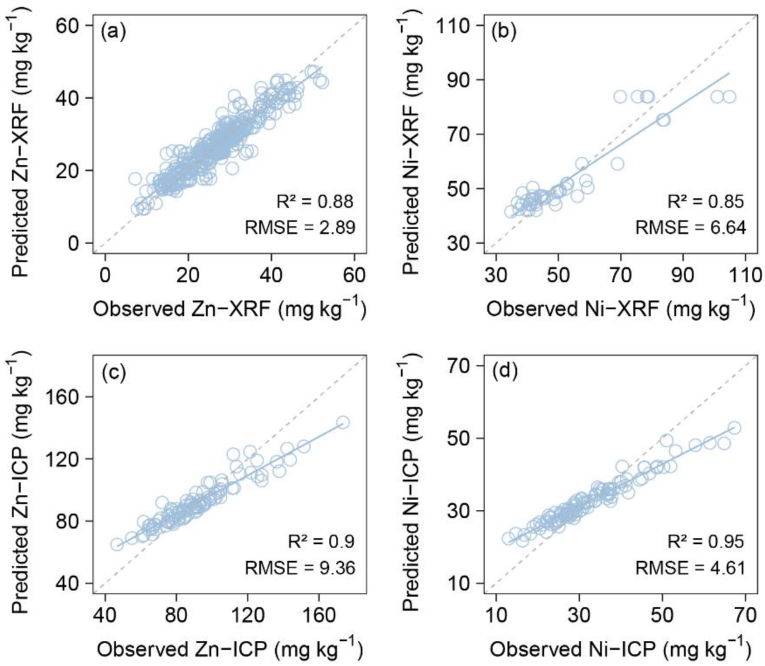

Figure R2. XRF-based observed values are highly correlated with the XRF-based predicted values (a-b), and the ICP-MS-based observed values are also highly correlated with the ICP-MS-based predicted values (c-d).

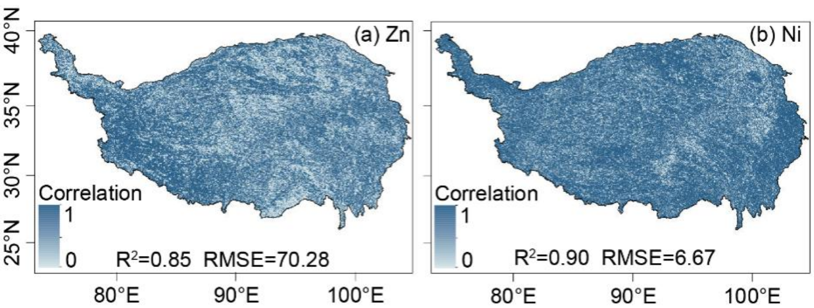

Figure R3. Spatial correlation maps of Zn and Ni contents before and after calibration of XRF measurements against ICP-MS. The strong consistency confirming that the calibration adjusted absolute contents but did not alter the large-scale spatial patterns of these elements.

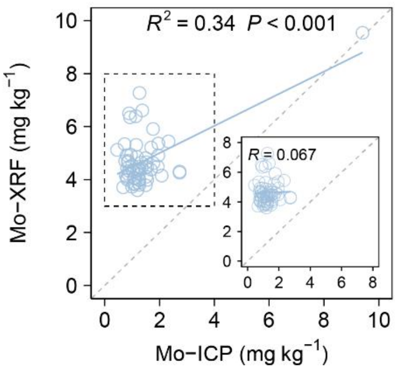

Figure R4. Comparison between laboratory-based third-generation XRF and ICP-MS measurements for Mo. The results obtained from the two methods were not fully consistent, likely due to its low content. The XRF-based measurements may involve considerable uncertainties. Therefore, we have included both the observational and predicted results in the supplementary materials and discussed their potential uncertainties in detail in the Discussion section.

[Comment 2] The use of relative importance metrics ('betasq') is a good start, but the analysis could be significantly strengthened. Consider using alternative methods (e.g., permutation importance from the Random Forest model itself) to cross-validate the reported driver rankings.

[Response] Following the suggestion, we complemented the relative importance analysis with Random Forest permutation importance to validate the driver rankings (**Figure R5**). Results showed that "*Soil properties were the primary contributors to the spatial variation of micronutrient contents, followed by topographic and climatic factors, whereas vegetation and grazing disturbance had relatively minor effects. Among all predictors, the Chemical Index of Alteration (CIA), slope, and soil texture exhibited the highest importance, indicating that weathering intensity, terrain, and* *soil physical structure are the dominant controls on the spatial distribution of soil micronutrients. Specifically, CIA emerged as the dominant factor for Fe, Zn, and V. Topographic factors (slope) primarily influenced Mn, while climatic variables (MAP, AI) and biological productivity (NPP) contributed more to Cu and Ni variations".* This result differs from that obtained using the 'betasq' relative importance metric, which is based on the assumption of a linear or approximately linear relationship between the response and predictor variables. In contrast, the Random Forest approach can capture complex non-linear and interactive effects among environmental variables. Considering that certain environmental factors may exert non-linear influences on micronutrient distributions, such as the observed U-shaped response to precipitation, we retained the permutation importance results derived from the Random Forest model in the updated version. The model's performance also improved by 3-52%, as indicated by the increase in R^2 from 0.25-0.54 ('betasq') to 0.39-0.77 ('Random Forest model').

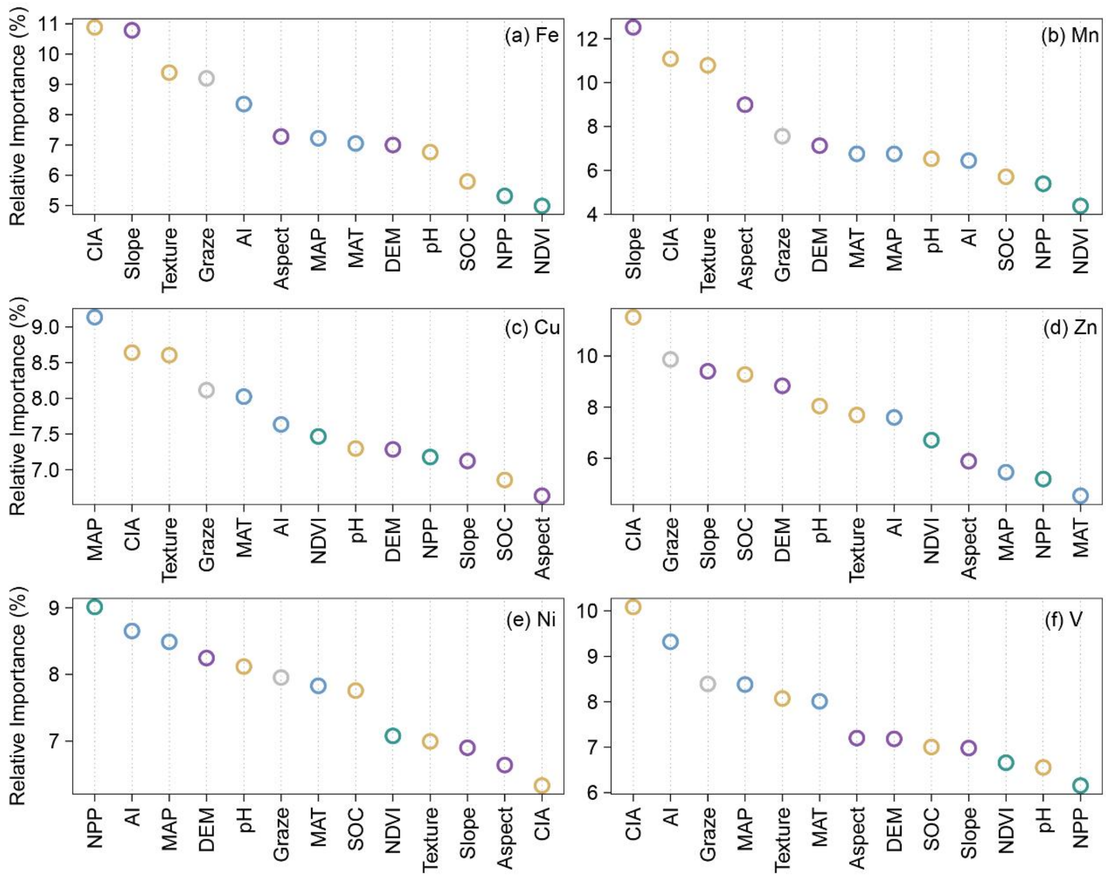

Figure R5. Relative importance of biotic and abiotic factors for soil micronutrients (Fe, Mn, Cu, Zn, Ni, V) on the Tibetan Plateau.

[Comment 3] Furthermore, the discussion of the U-shaped response to MAP (Line 191) is intriguing but remains qualitative. A more rigorous statistical exploration of these nonlinear relationships (e.g., using generalized additive models) would greatly bolster this key finding.

[Response] In the revision, we conducted a more rigorous statistical analysis using accumulated local effects (ALE) to characterize the nonlinear relationships between soil micronutrients and MAP (**Figure R6**). For Fe, Mn, Cu, Zn, and V, the response curves followed a decrease-stabilization-increase pattern, forming a clear U-shaped response. Predicted micronutrients decreased sharply under low to moderate precipitation, remained relatively stable across intermediate precipitation, and then increased again under high precipitation. Ni showed a hump-shaped pattern, with high values at low MAP followed by a gradual decline and subsequent stabilization. Both PDP and ALE analyses identified similar trends, confirming the robustness of the nonlinear precipitation effects on soil micronutrient distributions. This pattern likely reflects a trade-off between weathering, leaching losses and element retention under contrasting hydrological conditions. We have added these points into updated Discussion.

Here we chose ALE instead of GAMs because ALE captures conditional effects consistent with the Random Forest structure, avoiding biases from correlated or interacting predictors and better reflecting precipitation's nonlinear influence on micronutrients. Thanks for your understanding.

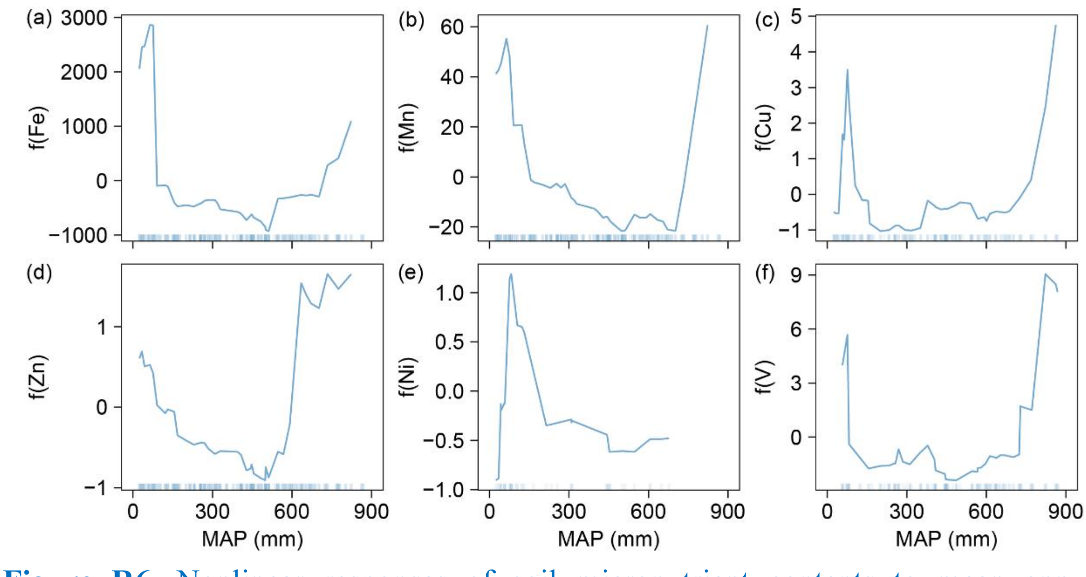

Figure R6. Nonlinear responses of soil micronutrient contents to mean annual precipitation (MAP) estimated with accumulated local effects (ALE). The short ticks (rugs) beneath each graph indicate the distribution density of the samples along the MAP axis.

[Comment 4] The poor performance of the models for Cu and Mo needs a more thorough discussion. Simply stating limited utility is insufficient. The authors should hypothesize why these elements are less predictable. Are the key drivers not captured in the predictor set? Is measurement error higher? Is their distribution more stochastic? This critical reflection is essential for a balanced interpretation of the results.

[Response] Thanks for the kind comment. In the revision, we added a subsection to discuss why Cu and Mo exhibit weaker predictive performance. First, analytical limitations may introduce measurement error, as both elements occur at very low contents. Second, key process controls are not fully captured by the current predictors. E.g. Cu is strongly influenced by nonlinear interactions with Fe/Al oxides, whereas Mo is affected by carbonate content, redox conditions (Tack et al., 1995). These mineralogical and redox variables are underrepresented, leading to potential bias. In addition, both elements show hotspot-prone, right-skewed distributions (**Figure 2**), likely due to localized anthropogenic sources. The spatial heterogeneity introduces stochastic variability beyond the range of our covariates. We have added these points into revised Discussion. Also, we added pixel-level uncertainty layers with the maps for users to properly utilize these datasets.

[Comment 5] The results show significant lithological control for some elements (Fig. 4), yet climate is reported as the dominant driver in the importance analysis (Fig. 5). This apparent discrepancy needs reconciliation. The discussion should integrate these findings, explaining how regional climate patterns might override or interact with the inherent geochemical signal from the parent material across the vast plateau.

[Response] Many thanks for this thoughtful comment. A closer examination of Fig. 4 shows that Fe, Mn, Zn, Ni, and V display slightly higher contents over acidic metamorphic rocks (MA), whereas Cu show no significant lithological differences (**Figure R7**). Although lithological differences are detectable for some elements, they do not alter the overall spatial patterns. The weak lithological signal for Cu further suggests limited parent-material control. In summary, lithology modulates the baseline levels of certain micronutrients but is not the dominant factor shaping their regional distributions, which are more strongly governed by external environmental drivers such as climate, weathering intensity, sediment transport, and biotic cycling. We have incorporated these points into the revised Discussion.

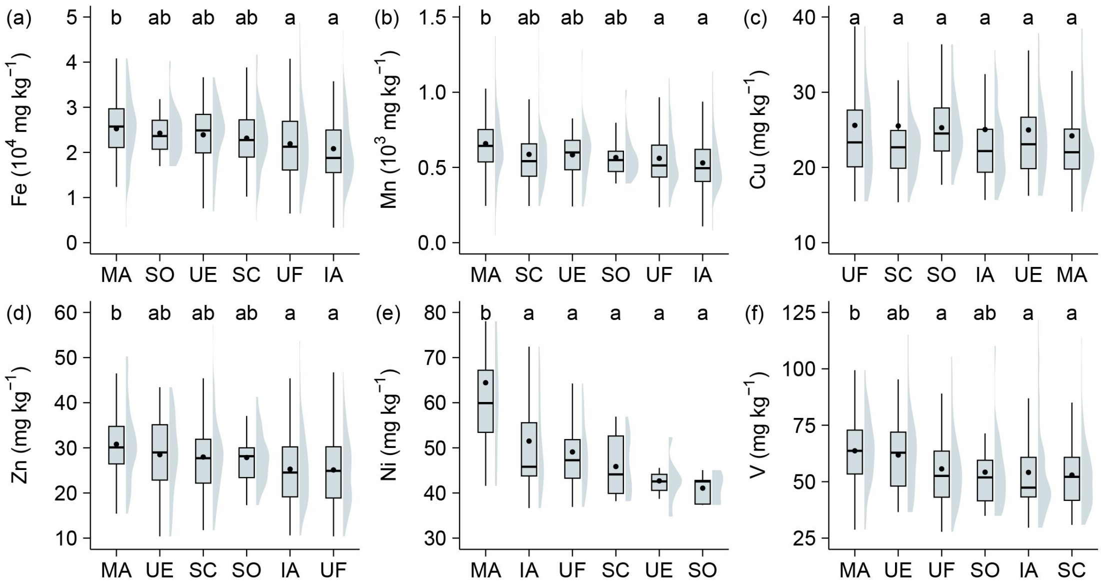

Figure R7. Variability in soil micronutrient contents (Fe, Mn, Cu, Zn, Ni, V) across Tibetan lithological classes. Abbreviations of lithological classes: IA = acidic igneous rock, MA = acidic metamorphic rock, SC = clastic sedimentary rock, SO = carbonate rock, UE = eolian facies rock, UF = fluvial facies rock.

[Comment 6] The high-resolution prediction maps (Fig. 7) are a key output. However, the manuscript does not provide associated uncertainty maps (e.g., prediction intervals). For users to properly utilize these datasets, an assessment and visualization of spatial uncertainty are crucial. Please add this or explicitly state it as a limitation.

[Response] Following your suggestion, we considered the model-based uncertainty from the Random Forest algorithm and added a pixel-level uncertainty layer (**Figure R8**) alongside the spatial prediction maps and supplemented the calculation method in the Methods section: "*The uncertainty layer is calculated as the inter-pixel variance among tree predictions*".

In addition, we discussed the input-data-related uncertainties not quantified in this study. The gridded climate data were derived based on a limited number of meteorological stations, and sparse coverage at high elevations may introduce biases in the western Plateau. Likewise, the soil property data, though based on all available field observations, remain limited in remote areas, potentially causing systematic bias. These data constraints still affect prediction accuracy of soil micronutrients. Accordingly, we added the following statement to the revised manuscript: *"The spatial predictions inevitably contain uncertainties arising from both the Random Forest model and the input datasets. Model-based uncertainty was quantified as the inter-tree variance among predictions, while additional uncertainty may stem from sparse meteorological observations and limited soil sampling across the Tibetan Plateau"*.

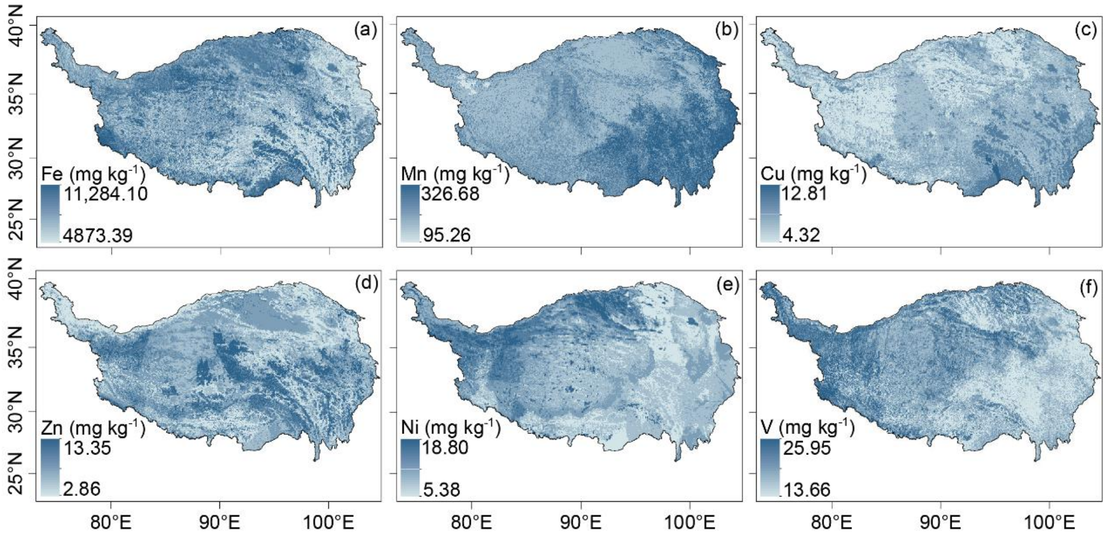

Figure R8. Spatial uncertainty of soil micronutrients (Fe, Mn, Cu, Zn, Ni, V) predictions across the Tibetan Plateau, expressed as standard deviation of per-tree predictions in the random forest; units in mg kg^{-1}.

Minor Comments:

[Comment 7] The abstract mentions six microelements but the title and data availability specify only four (Fe, Mn, Zn, Ni). The title and abstract should be aligned. Either adjust the title to reflect the full study or refocus the abstract on the four well-predicted elements.

[Response] We have updated the title as follows: *"Mapping key soil micronutrients across the Tibetan Plateau"*.

[Comment 8] Figure 1b is described but not effectively explained in the caption. The relationship between the bars and dots (ecosystem area vs. sampling frequency) should be explicitly stated to justify the representativeness of the sampling strategy.

[Response] We have revised the caption of Fig. 1b to state that the bars represent the areal proportion of each ecosystem, while the dots represent the proportion of sampling sites within the same ecosystem. Similar bar and dot heights indicate that the sampling is proportionally representative.

[Comment 9] The terms "micronutrients," "microelements," and "trace elements" are used interchangeably. For consistency and precision, authors should choose the same word throughout the manuscript.

[Response] To ensure consistency and precision, we use "micronutrients" throughout the manuscript.

[Comment 10] The data availability section provides a DOI, but this should also be formally cited in the main text (e.g., in the Methods or Results section) when the dataset is first mentioned.

[Response] We have added a formal citation with the DOI at the first mention of the dataset in the Abstract section.

[Comment 11] Line 40 has a trailing comma after "Mo" ("...Ni, Mo,).").

[Response] The redundant comma has been deleted.

[Comment 12] The discussion on ecological implications (Lines 228-233) is good but could be slightly expanded. Briefly mention specific plateau processes that might be most sensitive to these micronutrient limitations.

[Response] Thank you for the suggestion. Multiple biogeochemical processes are sensitive to micronutrient availability. Biological nitrogen fixation relies on Mo and Fe as essential cofactors of nitrogenase, while the methane cycle depends on Ni and Cu through their roles in methanogenesis and methane oxidation, respectively (Thauer et al., 2019; Stefan et al., 2020). Permafrost thaw and thermokarst development can further activate Fe-Mn redox cycling, altering metal mobility (Chauhan et al., 2024). Collectively, soil micronutrients depletion may cascade through nutrient cycling and ecosystem feedbacks, amplifying the impacts of ongoing environmental change across the Plateau. We have incorporated these points into revised Discussion.

In the end, we would like to express our sincere gratitude to the reviewer once again for the valuable time, effort, and constructive feedback that have greatly helped improve the quality of our manuscript.

References:

Chauhan, A., Patzner, M. S., Bhattacharyya, A., Borch, T., Fischer, S., Obst, M., Thomasarrigo, L.K., Kretzschmar, R., Mansor, M., Bryce, C., Kappler, A., and Joshi, P.: Interactions between iron and carbon in permafrost thaw ponds, Science of the Total Environment, 946, 174321, https://doi.org/10.1016/j.scitotenv.2024.174321, 2024.

Lemière, B.: A review of pXRF (field portable X-ray fluorescence) applications for applied geochemistry, Journal of Geochemical Exploration, 188, 350-363, https://doi.org/10.1016/j.gexplo.2018.02.006, 2018.

Simon M. N.: Inductively Coupled Plasma Mass Spectrometry Handbook, Blackwell Publishing, Oxford, 2005.

Stefan, B., Jiménez-Vicente, E., Echavarri-Erasun, C., and Rubio, L. M.: Biosynthesis of Nitrogenase Cofactors, Chemical Reviews, 120, 4919-5794, https://doi.org/10.1021/acs.chemrev.9b00489, 2020.

Tack, F.M., Verloo M.G.: Chemical speciation and fractionation in soil and sediment heavy metal analysis: a review, International Journal of Environmental Analytical Chemistry 59, 225-238. https://doi:10.1080/03067319508041330, 1995.

Thauer, P. K.: Methyl (Alkyl)-Coenzyme M Reductases: Nickel F-430-Containing Enzymes Involved in Anaerobic Methane Formation and in Anaerobic Oxidation of Methane or of Short Chain Alkanes, Biochemistry, 58, 5198-5220. https://doi:10.1021/acs.biochem.9b00164, 2019.