



Integrating AI and biomimetic design for heavy metal remediation inspired by *Eichhornia crassipes*

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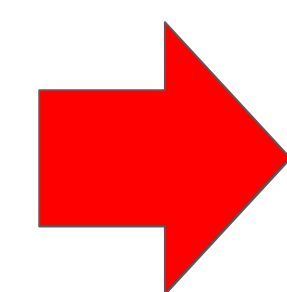
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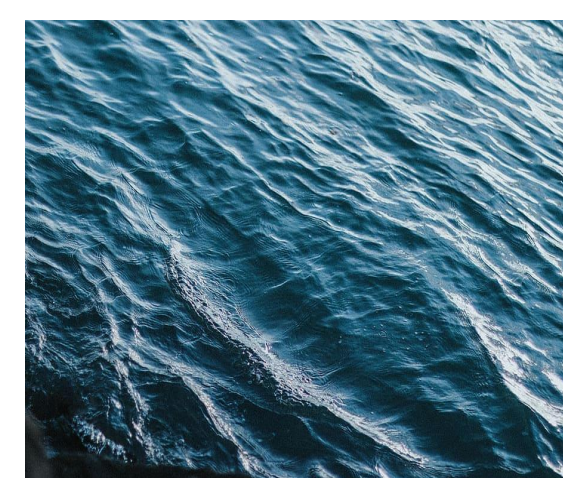
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Research Problem

Pb
Cd



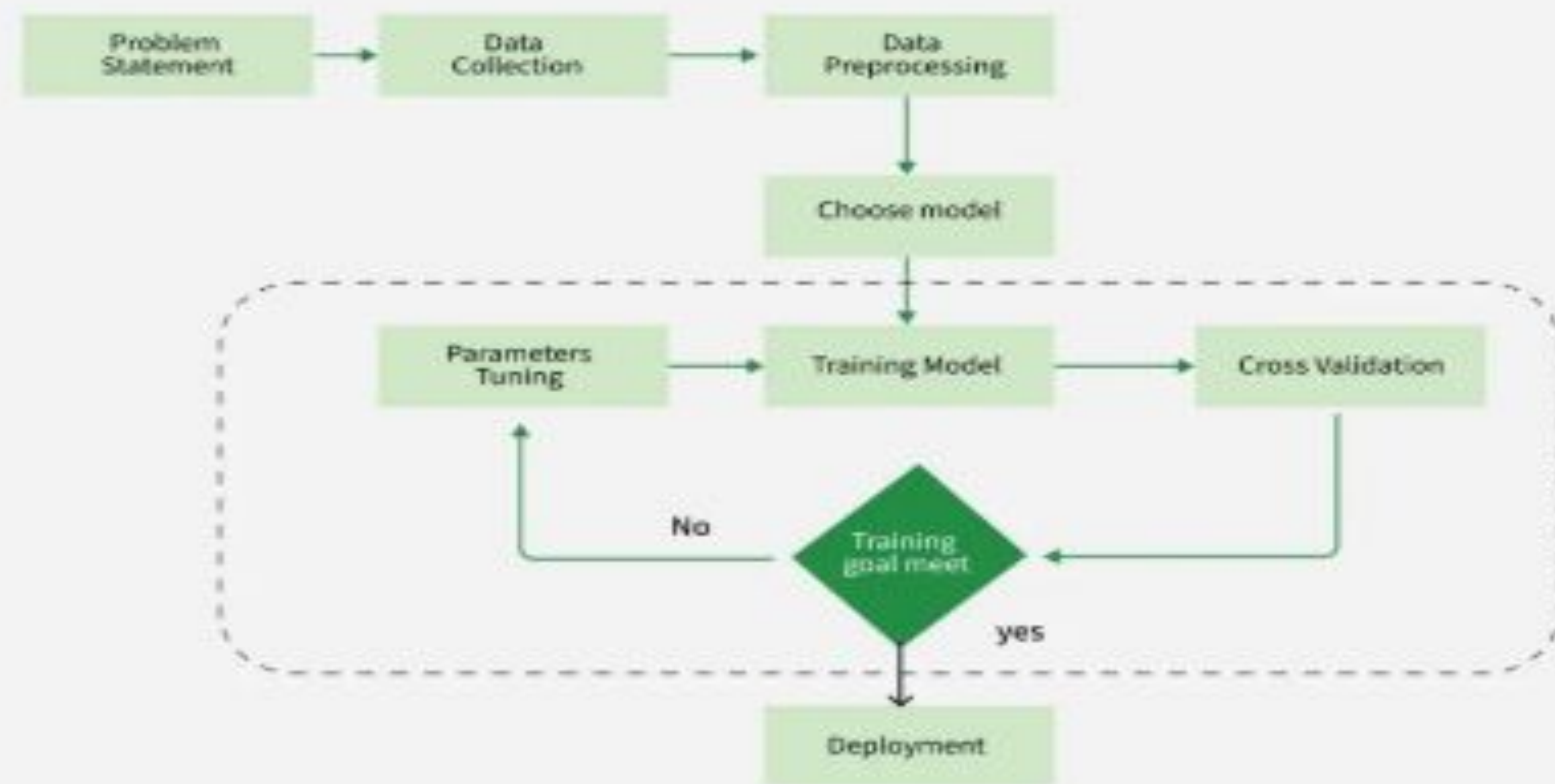
Polluted water



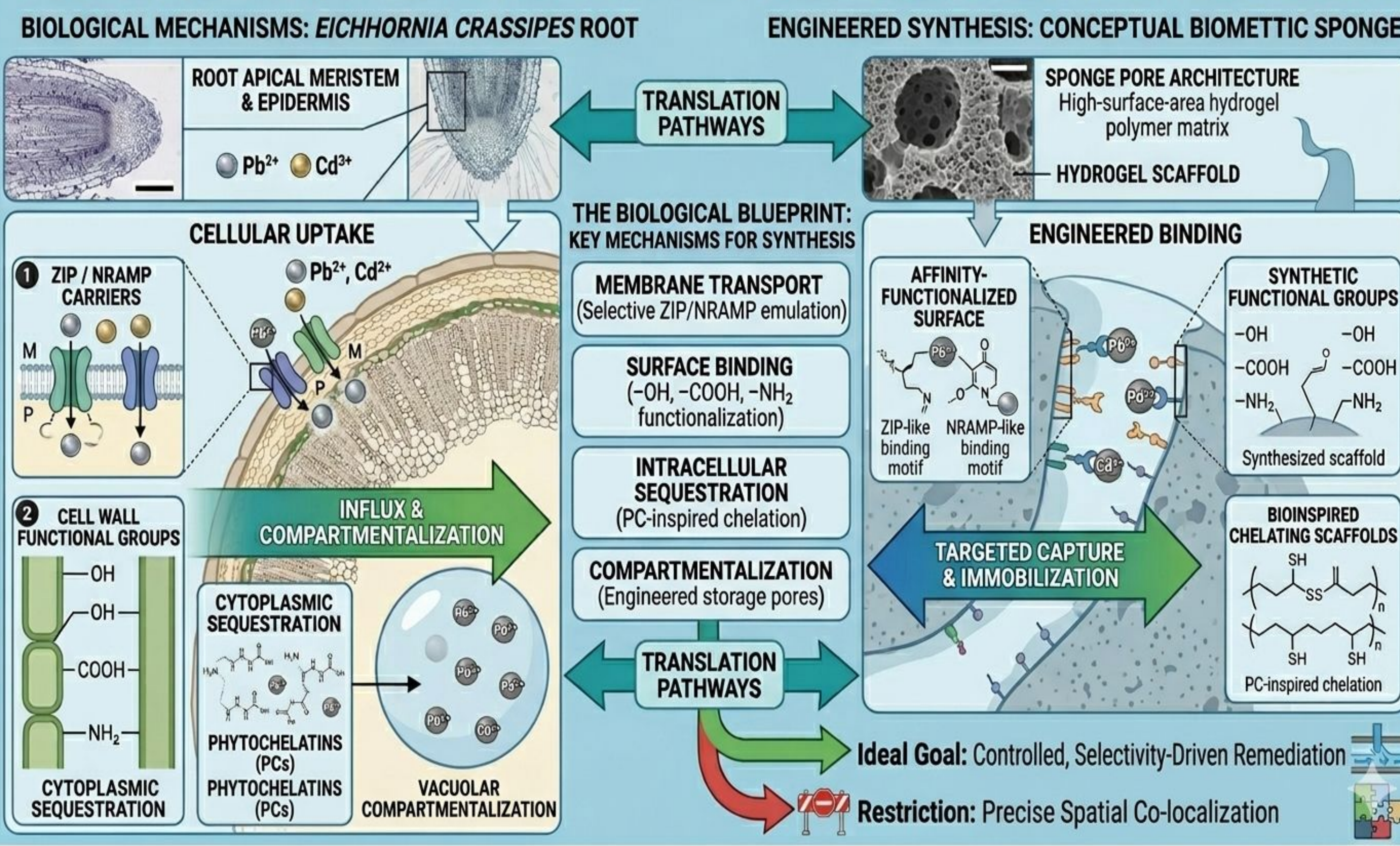
Main Objective

- To present a literature-based and concept-driven exploration of how the molecular mechanisms underlying *E. crassipes* metal uptake can be translated into engineered, biomimetic systems.
- To design synthetic systems that mimic biological metal binding while completely avoiding the ecological risks associated with using live, invasive plants.

Flowchart of Machine Learning Model



CONCEPTUAL BIOMETRIC SPONGE MODEL: SYNTHESIZING BIOLOGICAL MECHANISMS.



Integrated Methodology & Conceptual Framework

Spectroscopic Tools: Utilizing FTIR and NMR spectroscopy techniques to explicitly characterize and understand functional group interactions with metal ions.

Computational Modeling: Applying basic molecular modeling and Density Functional Theory (DFT) calculations to estimate the relative binding affinities of different functional groups.

Artificial Intelligence (AI): Deploying simple machine learning models (e.g., regression or classification based on small datasets) to predict trends in metal-ligand interactions and guide targeted material design.

Proposed Biomimetic Solution

- Platform:** A conceptual, highly controlled biomimetic system engineered as a functionalized polymer or hydrogel filter.
- Design:** Incorporates the key plant-inspired chemical binding motifs
- Capabilities:** Enables highly selective, efficient adsorption of heavy metals in a fully controlled and reusable format.
- Validation Status:** This work serves as an educational, non-experimental framework highlighting how biological principles inform sustainable engineering design.

Conclusion

Demonstrates how combining environmental chemistry, computational tools, and emerging AI approaches can drive next-generation remediation strategies.

Future Directions

Experimental Validation: Translating the literature-based, computational concept into laboratory reality by synthesizing and testing the physical functionalized hydrogel polymer.

Competitive Adsorption Studies: Testing how well the plant-inspired filter selectively traps Pb and Cd when mixed with other competitive ions naturally found in environmental water samples.

Scaling and Multi-Contaminant Expansion: Expanding the predictive machine learning models to guide the design of filters that can trap other heavy metals or organic industrial pollutants simultaneously.

References

- Mishra, V. K.; Tripathi, B. D. *Heavy metal accumulation in aquatic macrophytes and its role in phytoremediation*. *J. Environ. Biol.* 2008, 29, 27–32.
- Ali, H.; Khan, E.; Sajad, M. A. *Phytoremediation of heavy metals—Concepts and applications*. *Chemosphere* 2013, 91, 869–881.