Environment and Natural Resources Trust Fund

2027 Request for Proposal

General Information

Proposal ID: 2027-108

Proposal Title: Biochar-Based Solutions for Forever Chemical Contamination

Project Manager Information

Name: Joshua Layfield

Organization: University of St. Thomas

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Project Basic Information

Project Summary: Treatment solutions for contaminated water in Minnesota will be advanced through the development of computer simulation models of molecular-level interactions between PFAS and biochar interfaces.

ENRTF Funds Requested: $124,000

Proposed Project Completion: June 30, 2030

LCCMR Funding Category: Small Projects (G)

Secondary Category: Water (B)

Project Location

What is the best scale for describing where your work will take place?

Statewide

What is the best scale to describe the area impacted by your work?

Statewide

When will the work impact occur?

During the Project and In the Future

Narrative

Describe the opportunity or problem your proposal seeks to address. Include any relevant background information.

Since PFAS were first discovered in Minnesota waters in the early 2000s, researchers and state agencies have been working to address the "forever chemical" problem. The state's PFAS Blueprint identifies ten priorities for addressing the health and environmental challenges posed by PFAS, including remediating PFAS-contaminated sites. Remediation is especially challenging because the strong carbon-fluorine bonds and ionic character of PFAS render them resistant to microbial breakdown and thermal and photodegradation. The current state-of-the-art method to remove PFAS from water is granular activated carbon (GAC), which requires significant energy and financial inputs to produce.
Biochar is a carbon-rich material similar to GAC, produced by heating wood or crop waste in a low-oxygen environment at significantly lower cost. It has shown strong potential for removing PFAS from water, and Minnesota is investing in biochar research and production statewide. However, a critical knowledge gap remains: we do not fully understand why some biochars capture PFAS better than others. The temperature used to make biochar, its surface chemistry, and minerals dissolved in Minnesota water all affect performance, but the underlying molecular reasons are poorly understood. Without this knowledge, biochar optimization relies on expensive trial and error.

What is your proposed solution to the problem or opportunity discussed above? Introduce us to the work you are seeking funding to do. You will be asked to expand on this proposed solution in Activities & Milestones.

We propose to address that knowledge gap using molecular dynamics (MD) simulations to investigate how PFAS compounds attach to biochar surfaces at the molecular scale. MD simulations track interacting molecules over time like a molecular movie, providing atomic-level detail unavailable from experiments. From these simulations, we will calculate the structure, motion, and interaction energies between PFAS molecules and biochar surfaces, comparing surfaces prepared under different conditions to optimize PFAS capture.
The project will investigate three factors that govern real-world biochar performance. First, we will examine how production temperature changes the surface's ability to bind PFAS. Second, we will study how oxygen-containing surface groups on the biochar (which can be controlled by the amount of oxygen available in the heating phase) affect PFAS removal across the pH range of Minnesota waters. Third, we will investigate how dissolved mineral ions in Minnesota groundwater interact with biochar surfaces and influence PFAS capture.
Together, these three factors will produce a molecular-level picture of how biochar captures PFAS, and how production can be optimized for Minnesota's specific water conditions and target contaminants. Results will support groundwater remediation efforts by allowing Minnesota biochar producers to develop more effective, site-specific PFAS removal materials.

What are the specific project outcomes as they relate to the public purpose of protection, conservation, preservation, and enhancement of the state’s natural resources?

This project will support the protection and preservation of Minnesota's water resources by advancing a sustainable, low-cost treatment solution for PFAS-contaminated groundwater and surface water. We will accomplish this goal by producing a molecular-level understanding of PFAS adsorption on biochar, providing actionable guidance for optimizing biochar production for Minnesota water remediation. Key outcomes include simulation datasets showing how pyrolysis temperature, oxygen content, and dissolved ions alter biochar surface chemistry and affect PFAS capture; and a peer-reviewed publication and public presentations to make findings widely available. All datasets will be made publicly accessible in online repositories.

Activities and Milestones

Activity 1: Investigate the Role of Biochar Production Temperature on PFAS Interactions

Activity Budget: $39,438

Activity Description:
Objective:
Determine how the temperature used to produce biochar — which controls its pore structure and surface chemistry — affects its ability to capture PFAS molecules from water.
Tasks and Approach:
Four representative biochar surface models will be constructed corresponding to production temperatures of 300°C, 400°C, 500°C, and 700°C — the realistic range used by Minnesota producers, including the Natural Resources Research Institute (NRRI) facility in Coleraine. These models will capture the key structural differences temperature creates: lower-temperature biochars retain more oxygen-bearing surface groups (hydroxyl and carboxyl), while higher-temperature biochars develop larger pore sizes and more graphene-like carbon sheets. MD simulations will be run for each surface model in the presence of water and three PFAS compounds commonly detected in Minnesota — PFOA, PFOS, and PFBS — measuring the strength and speed of PFAS attachment to each surface type.
Outputs:

- Quantitative binding energies and attachment rates for each temperature-surface combination
- A ranking of production temperatures for PFAS capture effectiveness, with mechanistic explanations
- Molecular visualizations and a technical report for Minnesota biochar producers

Activity Milestones:

Description	Approximate Completion Date
Biochar surface models constructed for all four temperature conditions	August 31, 2027
MD simulations completed for PFOA, PFOS, and PFBS on all four surfaces	December 31, 2027
Binding energy and adsorption mechanism analysis completed	June 30, 2028

Activity 2: Investigate the Role of Biochar Oxygen Content and pH on PFAS Capture

Activity Budget: $41,663

Activity Description:
Objective:
Understand how oxygen-containing chemical groups on the biochar surface — which determine its surface charge — affect PFAS removal across the range of pH levels found in Minnesota groundwater and surface water.
Tasks and Approach:
Building on the framework from Activity 1, biochar surface models will be constructed with systematically varied oxygen functional group compositions: surfaces dominated by hydroxyl (–OH) groups, carboxyl (–COOH) groups, carbonyl (C=O) groups, and a control surface with minimal oxygen. Minnesota waters span a pH range of roughly 6.5 to 8.5; at different pH levels, these surface groups carry different electrical charges, altering how PFAS molecules — which carry negative charges at environmental pH — interact with the surface. This activity also examines how structural changes linked to oxygen content, such as pore size and surface hydrophobicity, affect PFAS capture. Simulations will be performed across this pH range for each surface type.
Outputs:

- Data identifying which oxygen functional groups most strongly attract PFAS under Minnesota water chemistry conditions.

- A pH-performance relationship usable by water treatment operators to predict biochar effectiveness
- Recommendations for surface modification strategies that enhance PFAS removal.

Activity Milestones:

Description	Approximate Completion Date
Oxygen-functionalized biochar surface models constructed and validated	July 31, 2028
Simulations completed across pH range for each surface type	December 31, 2028
pH-performance relationship analysis and structural change assessment completed	June 30, 2029

Activity 3: Investigate the Association of Cations with Negatively Charged Biochar Surfaces

Activity Budget: $42,899

Activity Description:

Objective:

Determine how dissolved mineral ions — especially calcium (Ca^{2+}) and magnesium (Mg^{2+}) that are abundant in Minnesota groundwater — interact with negatively charged biochar surfaces and how their presence helps or hinders PFAS capture.

Tasks and Approach:

Minnesota groundwater is commonly 'hard' — rich in dissolved calcium and magnesium. These positively charged ions are attracted to the same negatively charged sites on biochar that PFAS molecules target. This competition could reduce PFAS capture, or alternatively, these ions may form bridges between the biochar surface and PFAS, enhancing removal. MD simulations will model biochar surfaces immersed in solutions representing realistic Minnesota groundwater mineral concentrations, tracking how Ca^{2+}, Mg^{2+}, Na^{+}, and K^{+} ions distribute around the surface, compete with PFAS for binding sites, and alter the overall electrostatic environment at the surface. Both short-chain (PFBS) and long-chain (PFOS, PFOA) PFAS will be tested, since shorter-chain compounds are generally harder to remove and of particular regulatory concern in Minnesota.

Outputs:

- Molecular-level understanding of competitive and cooperative effects between cations and PFAS at biochar surfaces
- Ion concentration thresholds above which water hardness degrades biochar PFAS removal performance
- Recommendations for water pre-treatment or biochar surface modification to maintain effectiveness in Minnesota's hard water

Activity Milestones:

Description	Approximate Completion Date
Minnesota groundwater chemistry parameters compiled; ion force fields validated	June 30, 2029
Simulations with Ca^{2+}/Mg^{2+}/Na^{+}/K^{+} at representative concentrations completed	August 31, 2029
Competitive binding analysis for short-chain vs. long-chain PFAS completed	June 30, 2030

Dissemination

Describe your plans for dissemination, presentation, documentation, or sharing of data, results, samples, physical collections, and other products and how they will follow ENRTF Acknowledgement Requirements and Guidelines.
Results from this project will be disseminated through multiple channels to ensure findings reach both the scientific community and the Minnesota stakeholders best positioned to act on them.
Peer-reviewed publications will be submitted to widely accessible journals in computational and environmental chemistry. Simulation datasets will be deposited in a public repository such as Zenodo to ensure long-term accessibility and reproducibility.
The project team will present findings at regional and national scientific conferences, including meetings of the American Chemical Society. We will also seek opportunities to present directly to applied stakeholders including the University of Minnesota's Natural Resources Research Institute, the Minnesota Pollution Control Agency, and Minnesota biochar producers. These presentations will translate simulation results into practical guidance for optimizing biochar production for specific water chemistry conditions found across Minnesota.
At the University of St. Thomas, undergraduate student researchers will participate directly in the project and will present their work at UST's annual research symposium and at the annual Associated Colleges of the Twin Cities chemistry conference. Plain-language summaries of findings will be shared through the UST Department of Chemistry website and through public outreach events.
All publications, presentations, reports, and outreach materials produced with support from this grant will acknowledge the Environment and Natural Resources Trust Fund in accordance with ENRTF Acknowledgment Guidelines, including use of the trust fund logo on all relevant print and electronic communications.

Long-Term Implementation and Funding

Describe how the results will be implemented and how any ongoing effort will be funded. If not already addressed as part of the project, how will findings, results, and products developed be implemented after project completion? If additional work is needed, how will this work be funded?
Simulation findings will be shared through peer-reviewed publications that will open opportunities to directly collaborate with experimental researchers and biochar producers. These studies will strengthen future funding applications to federal sources including NSF, USDA, and EPA. The undergraduate students at the University of St. Thomas who participate in this work will be trained as researchers with skills and interests that focus on Minnesota-specific issues. Students who continue to graduate school will carry Minnesota-focused PFAS remediation research forward.

Project Manager and Organization Qualifications

Project Manager Name: Joshua Layfield

Job Title: Associate Professor

Provide description of the project manager's qualifications to manage the proposed project.
Dr. Joshua Layfield has worked at the University of St. Thomas in the Department of Chemistry in St. Paul, Minnesota since 2014. His research focuses on molecular dynamics (MD) simulations of chemical systems at complex interfaces, with particular emphasis on developing and applying computational methods to study how molecules interact at surfaces and in condensed-phase environments. His doctoral dissertation examined the structure and dynamics of water confined between hydrophobic surfaces using MD simulations, work directly relevant to modeling PFAS behavior near carbonaceous adsorbents such as biochar. He has published 12 papers in the peer-reviewed literature in leading journals including the Proceedings of the National Academy of Sciences, the Journal of the American Chemical Society, and

Chemical Reviews. He has mentored more than thirty-five undergraduate researchers in computational chemistry through the University of St. Thomas and is committed to integrating students directly into research addressing real environmental challenges facing Minnesota.

Organization: University of St. Thomas

Organization Description:
The University of St. Thomas is Minnesota's largest private university, enrolling approximately 10,000 students across its campuses in St. Paul and Minneapolis, with a strong tradition of undergraduate research and community-engaged scholarship (https://www.stthomas.edu). The Department of Chemistry provides the project manager with dedicated office space and high-performance computing access through a departmental cluster and the Minnesota Supercomputing Institute — the computational infrastructure needed to carry out the proposed molecular dynamics simulations. This work reflects the university's broader mission: "Inspired by Catholic intellectual tradition, the University of St. Thomas educates students to be morally responsible leaders who think critically, act wisely, and work skillfully to advance the common good."

Budget Summary

Category / Name	Subcategory or Type	Description	Purpose	Gen. Ineligible	% Benefits	# FTE	Classified Staff?	$ Amount
Personnel								
Joshua Layfield		Project Manager			8%	0.51		$54,145
Student Researchers (2 per year, for 3 years)		Design, Setup, Perform, and Analyze Simulations			8%	1.71		$66,096
							Sub Total	**$120,241**
Contracts and Services								
							Sub Total	-
Equipment, Tools, and Supplies								
	Tools and Supplies	Hard Drives for Long-Term Data Storage	The data generated by the models will be preserved and made available by request on the research group's computer cluster. These simulations will generate approximately 50 TB of data and preserving the data will require additional hard drive space.					$1,759
							Sub Total	**$1,759**
Capital Equipment								
							Sub Total	-
Acquisitions and Stewardship								
							Sub Total	-
Travel In Minnesota								

	Conference Registration Miles/ Meals/ Lodging	Cost to attend a conference within the state to disseminate research results.	Attend a conference within the state of Minnesota to disseminate research results.					$2,000
							Sub Total	**$2,000**
Travel Outside Minnesota								
							Sub Total	**-**
Printing and Publication								
							Sub Total	**-**
Other Expenses								
							Sub Total	**-**
							Grand Total	**$124,000**

Classified Staff or Generally Ineligible Expenses

Category/Name	Subcategory or Type	Description	Justification Ineligible Expense or Classified Staff Request

Non ENRTF Funds

Category	Specific Source	Use	Status	Amount
State				
			State Sub Total	**-**
Non-State				
In-Kind	University of St. Thomas	Facilities and other expenses usually covered by indirect costs.	Potential	$51,336
			Non State Sub Total	**$51,336**
			Funds Total	**$51,336**

Total Project Cost: $175,336

This amount accurately reflects total project cost?

Yes

Attachments

Required Attachments

Visual Component

File: 7c21be61-ae5.pdf

Alternate Text for Visual Component

A diagram showing the three aspects of biochar to be investigated: 1) Carbon structure due to temperature, 2) the incorporation of oxygen defects, and 3) the presence of bound metal ions....

Financial Capacity

Title	File
UST Form 990	af2987c6-a07.pdf

Supplemental Attachments

Capital Project Questionnaire, Budget Supplements, Support Letter, Photos, Media, Other

Title	File
2027-108 letter of support UST_received 04-07-26	29f71835-34f.pdf

Administrative Use

Does your project include restoration or acquisition of land rights?

No

Do you understand that travel expenses are only approved if they follow the "Commissioner's Plan" promulgated by the Commissioner of Management of Budget or, for University of Minnesota projects, the University of Minnesota plan?

Yes, I understand the Commissioner's Plan applies.

Does your project have potential for royalties, copyrights, patents, sale of products and assets, or revenue generation?

No

Do you understand and acknowledge IP and revenue-return and sharing requirements in 116P.10?

N/A

Do you wish to request reinvestment of any revenues into your project instead of returning revenue to the ENRTF?

N/A

Does your project include original, hypothesis-driven research?

Yes

Does the organization have a fiscal agent for this project?

No

Does your project include the pre-design, design, construction, or renovation of a building, trail, campground, or other fixed capital asset costing $10,000 or more or large-scale stream or wetland restoration?

No

Do you propose using an appropriation from the Environment and Natural Resources Trust Fund to conduct a project that provides children's services (as defined in Minnesota Statutes section 299C.61 Subd.7 as "the provision of care, treatment, education, training, instruction, or recreation to children")?

No

Provide the name(s) and organization(s) of additional individuals assisting in the completion of this proposal:

Michael Warnock, UST

Do you understand that a named service contract does not constitute a funder-designated subrecipient or approval of a sole-source contract? In other words, a service contract entity is only approved if it has been selected according to the contracting rules identified in state law and policy for organizations that receive ENRTF funds through direct appropriations, or in the DNR's reimbursement manual for non-state organizations. These rules may include competitive bidding and prevailing wage requirements

N/A