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Sandia National Laboratories

NOVEL MATERIALS TO PRECONCENTRATE PFAS FOR ULTRA LOW DETECTION WITH LC-MS

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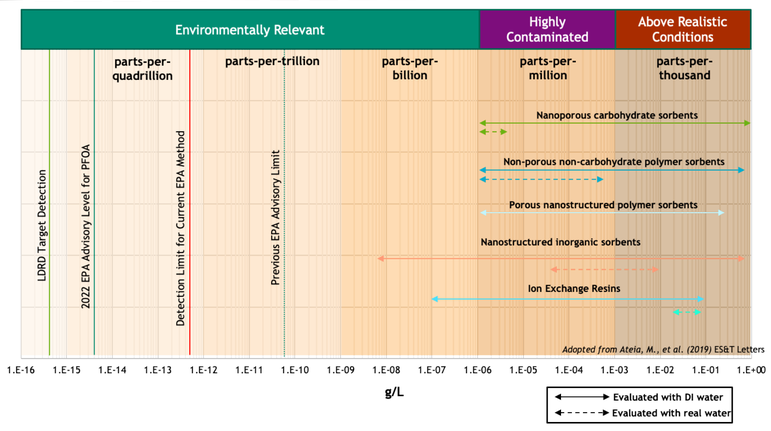
INTRODUCTION

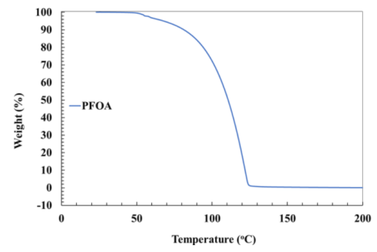
The *exceedingly low* EPA health advisory level (4 ppq) *necessitates* **a novel method to detect ultra-trace concentrations of PFAS** to assess the prevalence and environmental transport of PFAS, and provide safe drinking water.

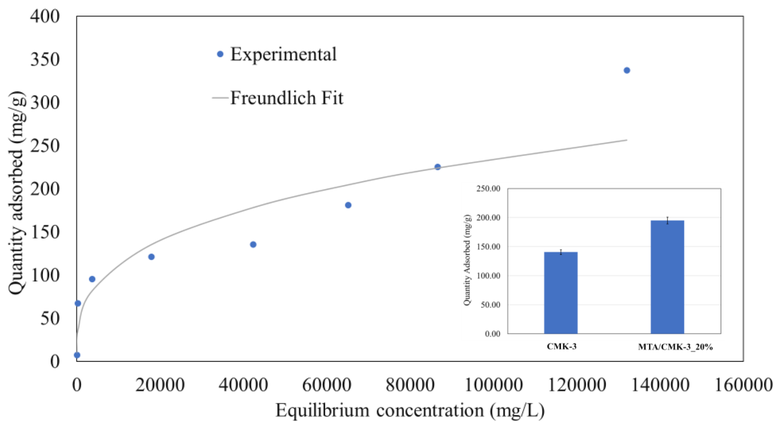


We *hypothesize* that preconcentrating PFOA on aliphatic quaternary amine functionalized carbon will allow for PFOA detection below the currently unreachable EPA limit using nano-LC-MS and improve our nation's ability to address this environmental crisis.

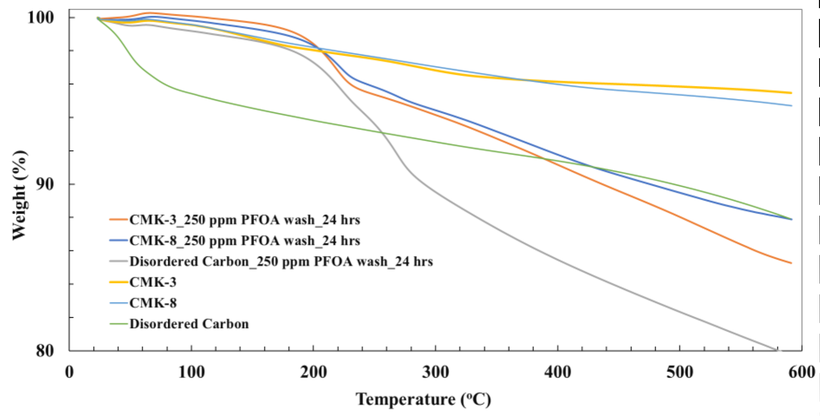
RESULTS

PFOA adsorption on a variety of functionalized carbonaceous substrates was confirmed by adsorption isotherms and TGA measurements. The functionalized materials showed a higher affinity toward PFOA than non-functionalized.





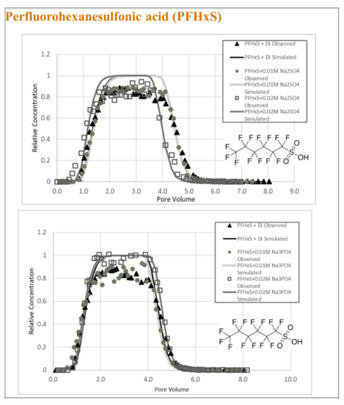
PFOA adsorption isotherm on CMK-3 fit to Freundlich model. Result of PFOA adsorption using 50 ppm of 50 mL solution

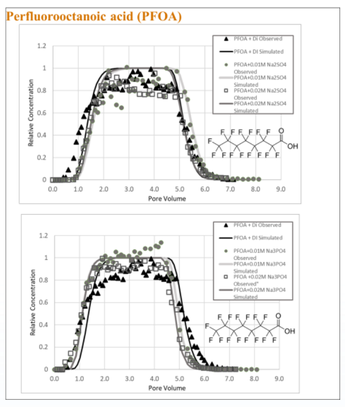


TGA of sorbents with and without PFOA, showing the onset of thermal degradation changes due to pore incorporation

University Partnership – NM State

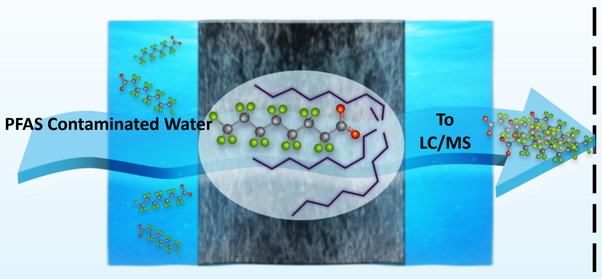
Evaluated competition adsorption on representative clay minerals with common anions at a wide range of initial PFAS concentrations. This allows for a better understanding of the concentrations specific surface complexation to improve our understanding PFAS competitive sorption and transport in soils and aquifers





CONCLUSION

Porous carbon materials functionalized with aliphatic quaternary amines have shown to be effective at pre-concentration PFOA. These materials could be very effective to aid in solid phase extraction efforts to detect PFOA down to the EPA health advisory level.



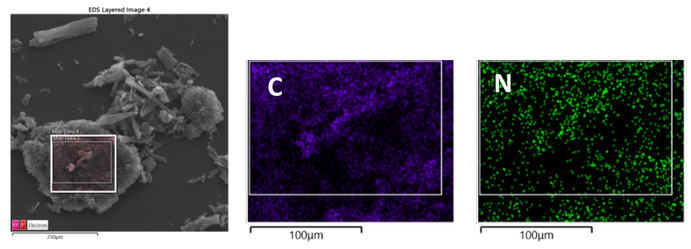
METHODOLOGY

Material Synthesis

Carbonaceous substrates were functionalized with aliphatic quaternary amines

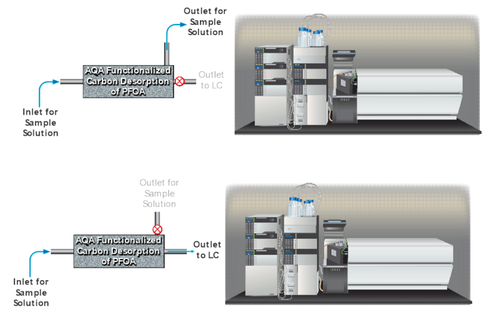
Substrate	Non-Functionalized		Adogen 464		Methyltrialkly ammonium chloride	
	Surface Area (m^2/g)	Pore Size (nm)	Surface Area (m^2/g)	Pore Size (nm)	Surface Area (m^2/g)	Pore Size (nm)
Disordered Carbon	575	4.8-9.1	16.38	NA	NA	NA
CMK-3	822	5.6-5.7	14.33	17.4-20.0	11.80	14.8-18.8
CMK-8	502	4.6-6.1	NA	NA	NA	NA

SEM of functionalized sorbent



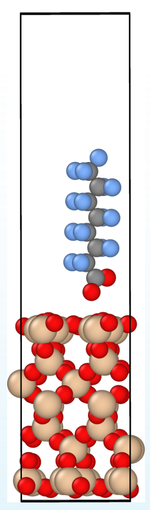
Adsorption and Desorption

Adsorption and desorption of PFOA will be evaluated to improve solid phase extraction process for quantification

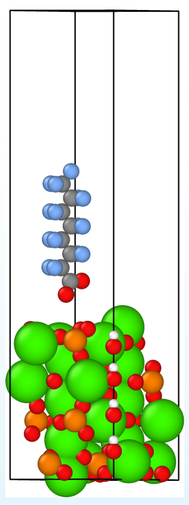


Computational Modeling

Atomistic simulation to understand PFOA adsorption on different mineral surfaces.



Alpha quartz



Hydroxyapatite

U.S. DEPARTMENT OF ENERGY
National Nuclear Security Administration

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