

Electronic Supporting Information (ESI)

Reversible adsorption and desorption of PFAS on inexpensive graphite adsorbents via alternating electric field

Bishwash Shrestha^{†,#}, *Mohammadamin Ezazi*^{†,#}, *Sanjay Ajayan*[†], and *Gibum Kwon*^{†,*}

[†] Department of Mechanical Engineering, University of Kansas, Lawrence, Kansas 66045, United States.

* Email: gkwon@ku.edu

These authors contributed equally

Calculation of specific capacitance, adsorption capacity, and adsorption rate.
Following equations were used to calculate the specific capacitance, adsorption capacity, and adsorption rate.

The specific capacitance (C) was calculated by¹:

$$(S1) C = \int I dV / 2UVm$$

where I , V , U , and m are the current, potential, the scan rate, and the mass of the electrodes, respectively.

The adsorption capacity (α) is defined as²:

$$(S2) \alpha = (C_o - C_t)Q / m$$

where C_0 and C_t (in ppm) are the concentration of PFAS solution at $t = 0$ and t , respectively. Q and m are the volume of the solution collected at the outlet of the cell and the mass of the anode, respectively.

The adsorption rate (R_a) was measured by²:

$$(S3) R_a = (C_o - C_t)Q / tA$$

where t and A are the time and the total surface area of the anode.

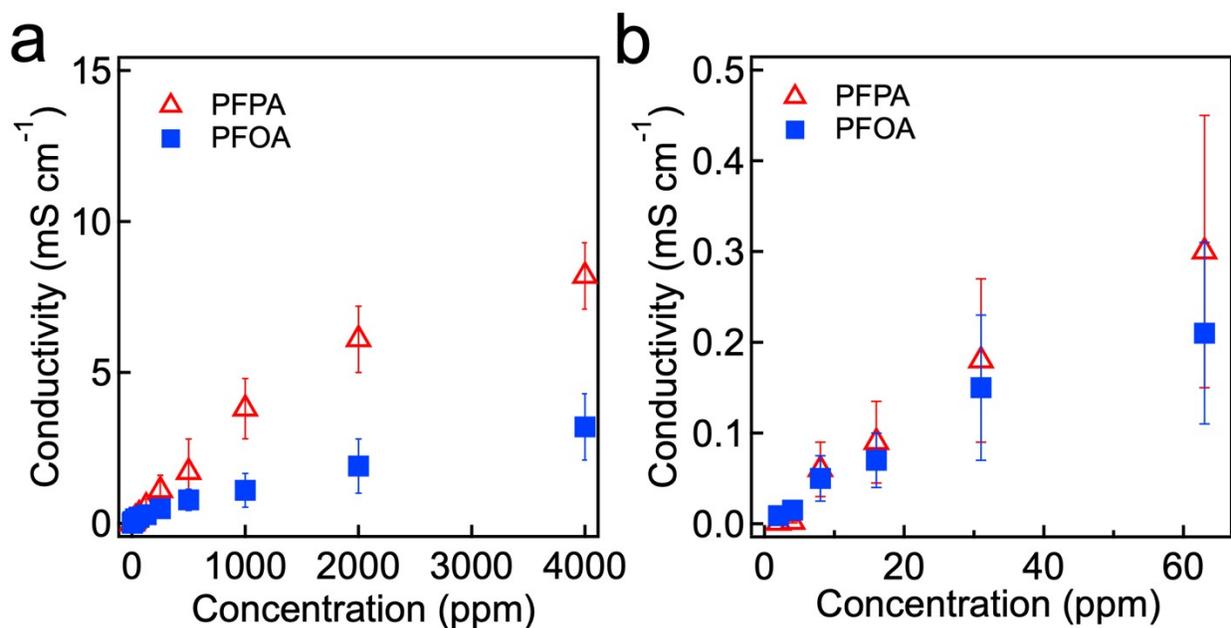


Figure S1. (a) and (b). The calibration curves established by calculating the electrical conductivity of DI water dissolved with PFPA (a) and PFOA (b) as a function of concentrations.

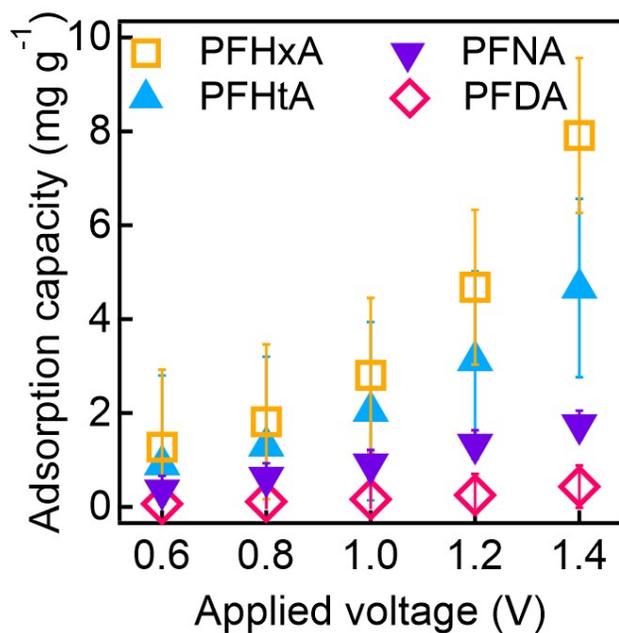


Figure S2. The measured adsorption capacity values for PFHxA, PFHtA, PFNA, and PFDA aqueous solutions at varied voltages. Note that the concentration (C_0) for each solution was 0.01 M. The adsorption capacity values are lower for PFAS with a longer fluoroalkyl chain.

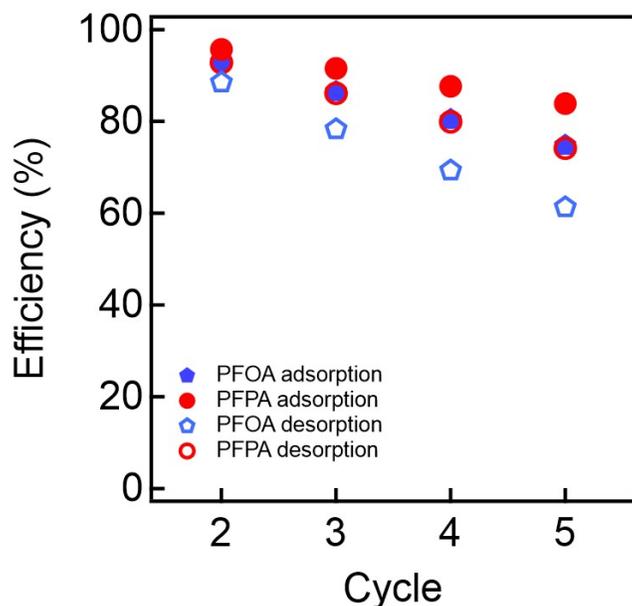


Figure S3. The measured adsorption and desorption efficiency as a function of cycles.

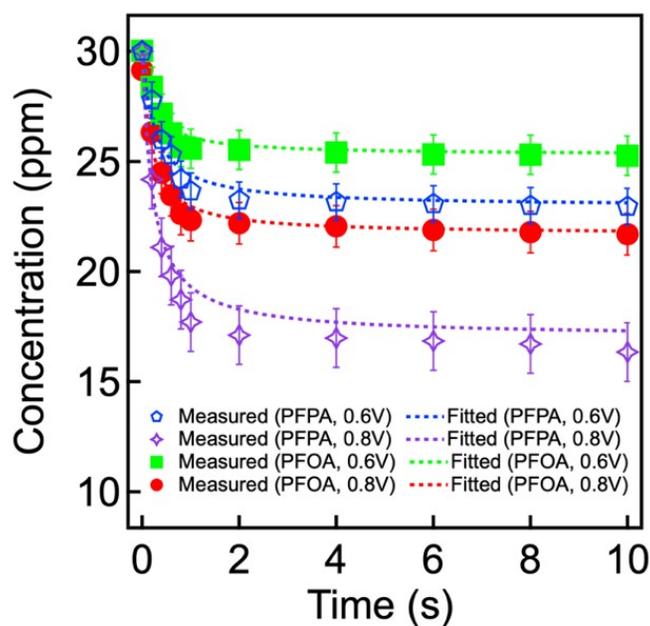


Figure S4. The measured concentrations for PFPA and PFOA aqueous solutions upon applying voltage of $V = +0.6$ V or $V = +0.8$ V. The fitted values of concentration utilizing pseudo-second order kinetic model for adsorption (**Eqn. 1** in main text) are also provided. The rate constants for adsorption (k_1) are determined as $k_1 = 0.3424 \text{ s}^{-1}$ ($V = +0.6$ V) and $k_1 = 0.5521 \text{ s}^{-1}$ ($V = +0.8$ V) for PFPA. For PFOA, we found $k_1 = 0.6723 \text{ s}^{-1}$ ($V = +0.6$ V) and $k_1 = 1.012 \text{ s}^{-1}$ ($V = +0.8$ V).

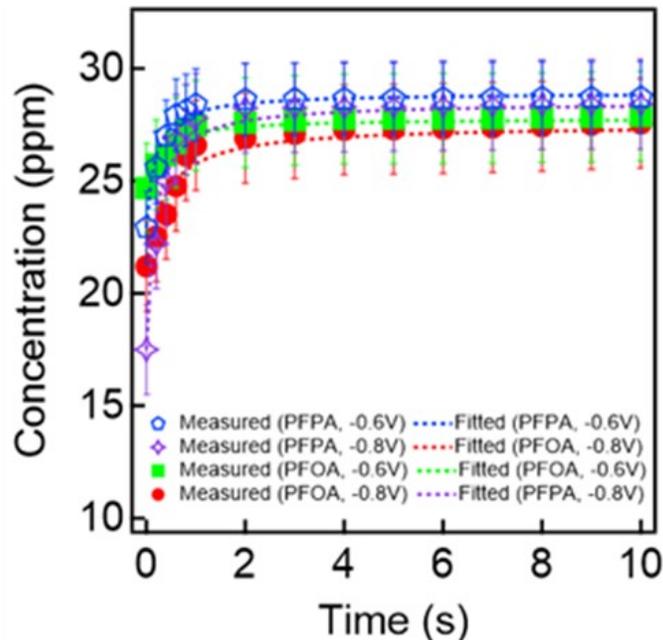


Figure S5. The measured concentrations for PFPA and PFOA aqueous solutions upon applying voltage of $V = -0.6$ V or $V = -0.8$ V. The fitted values of concentration utilizing pseudo-second order kinetic model for desorption (Eqn. 2 in main text) are also provided. The rate constants for desorption (k_2) are determined as $k_2 = 0.5553$ s⁻¹ ($V = -0.6$ V) and $k_2 = 0.9591$ s⁻¹ ($V = -0.8$ V) for PFPA. For PFOA, we found $k_2 = 0.417$ s⁻¹ ($V = -0.6$ V) and $k_2 = 1.19$ s⁻¹ ($V = -0.8$ V).

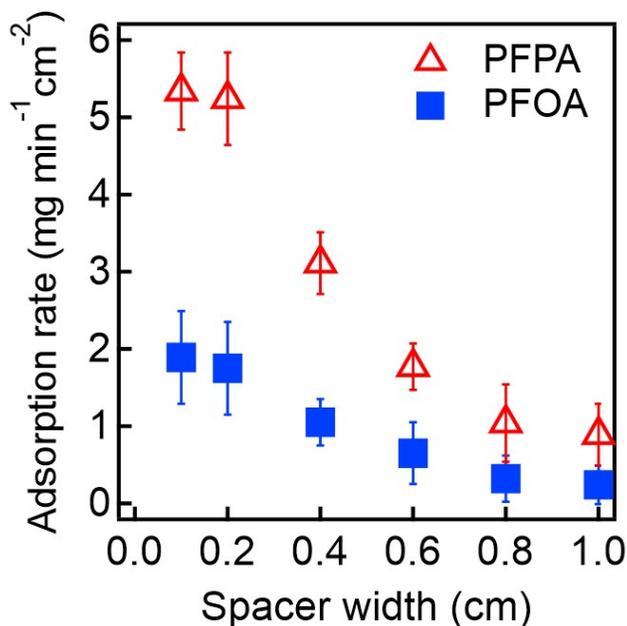


Figure S6. The measured adsorption rate (R_a) values of the module for PFPA and PFOA aqueous solutions ($C_o = 0.01$ M) as a function of the spacer width. It is observed that a spacer width of 0.2 cm exhibits the highest R_a values for both PFPA and PFOA.

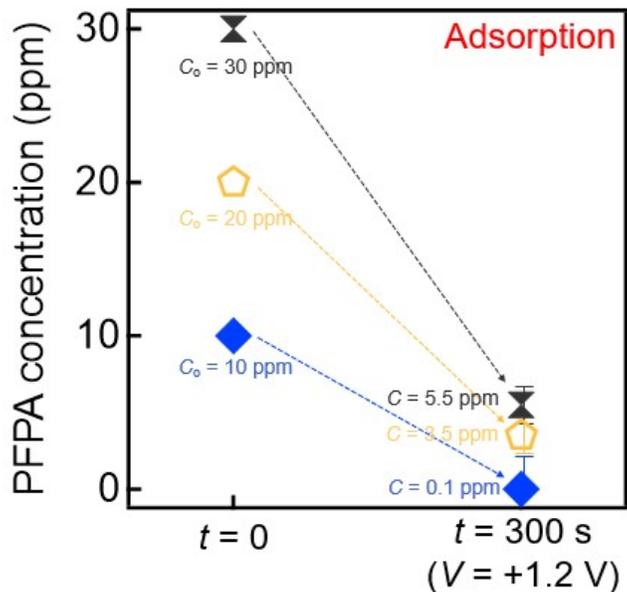


Figure S7. The measured concentrations of PFPA in the permeate after introducing 10 mL of feed PFPA solutions with varied concentrations ($C_0 = 30$ ppm, 20 ppm, and 10 ppm) to the device module.

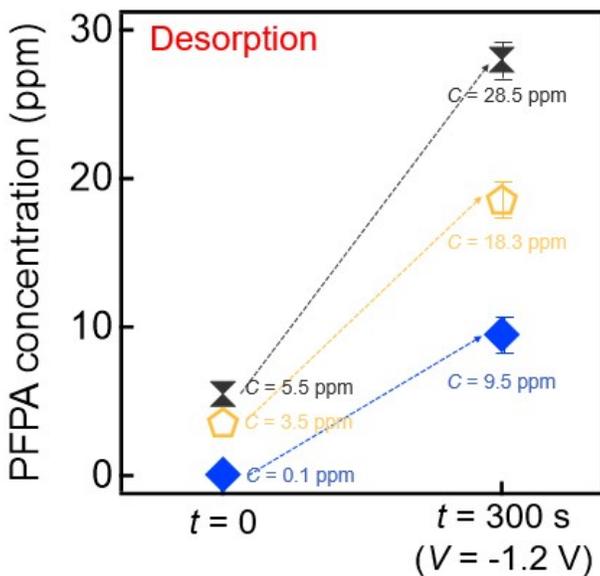


Figure S8. The measured concentrations of PFPA after desorption for solutions with varied initial concentrations ($C_0 = 30$ ppm, 20 ppm, and 10 ppm) utilizing the device module.

Table S1. The adsorption capacity (α) values of our graphite electrode for PFPA, PFHxA, PFHtA, PFOA, PFNA, and PFDA upon application of voltage ($V = + 1.2$ V). Note that all solutions are the same concentrations ($C_o = 0.01$ M). For comparison, the adsorption capacity values measured without application of voltage (i.e., conventional sorption) are also shown.

PFAS	Adsorption capacity (mg g ⁻¹)	
	With voltage	Without voltage
PFPA	10.20	0.20
PFHxA	4.87	0.12
PFHtA	3.36	0.07
PFOA	2.15	0.04
PFNA	1.56	0.031
PFDA	0.75	0.028

Reference

1. Z. Wang, B. Dou, L. Zheng, G. Zhang, Z. Liu and Z. Hao, *Desalination*, 2012, **299**, 96-102.
2. J. Han, T. Yan, J. Shen, L. Shi, J. Zhang and D. Zhang, *Environmental science & technology*, 2019, **53**, 12668-12676.