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Static iodine loading comparisons between activated carbons, zeolite, alumina, aerogel, and xerogel sorbents

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1 Sorbent Materials

Table S1. List of sorbent samples and abbreviated names used. AC denotes activated carbons, “d” and “l” denote diameter and length, respectively, and UNR and PNNL are University of Nevada, Reno and Pacific Northwest National Laboratory, respectively.

| # | Sorbents | Abbr. | Manufacturer/ Developer | Base Material | Impregnation Element/ Compound | Physical Form | Particle size (mm) | m_s (g) |
|----|---|-----------------------|----------------------------|------------------|--------------------------------------|---------------------------------|-------------------------|---------------------|
| 1 | Kombisorb BAT 37 | BAT37 | Donau Carbon | Carbon | S | Pellet | ~4 (d) × ~2-10 (l) | 1.7865 (±0.1495) |
| 2 | Kombisorb BAT II 37 | BAT37-II | Donau Carbon | Carbon | S | Pellet | ~3-4 (d) × ~2-10 (l) | 1.9125 (±0.0290) |
| 3 | 50% Desorex HGD 4S + 50% Oxorbon K 40 J | Des-Oxo | Donau Carbon | Carbon | KI | Pellet | ~3-4 (d) × ~2-10 (l) | 1.5866 (±0.1665) |
| 4 | 50% DARCO H ₂ S + 50% CABOT RBHG4 | Dar-Cab | Norit | Carbon | S | Unshaped particle, pellet | ~3-4 (d) × ~2-10 (l) | 1.6069 (±0.3165) |
| 5 | Carbon foam | CF | UNR | Carbon | None | Foam | – | 0.0205 (±0.0021) |
| 6 | IONEX-TYPE Ag 400 B3 | IONEX | Molecular Products | Aluminosilicate | Ag | Bead | 1-2 | 3.0654 (±0.1379) |
| 7 | AC6120 | AC6120 | Clariant | Alumina | Ag | Bead | 1.2-2.4 | 1.5268 (±0.0294) |
| 8 | Ag-functionalized aerogel | FA-Ag | PNNL | Silica | Ag | Unshaped particle | 1-5 | 1.1955 (±0.1106) |
| 9 | Ag-xerogel | HTX-Ag | PNNL | Aluminosilicate | Ag | Unshaped particle | 1-10 | 1.9317 |
| 10 | Ag-thiolated xerogel- reduced | HTX-S-Ag ⁰ | PNNL | Aluminosilicate | Ag, S | Unshaped particle | 1-10 | 0.1203 |
| 11 | Ag-thiolated xerogel- not reduced | HTX-S-Ag ⁺ | PNNL | Aluminosilicate | Ag, S | Unshaped particle | 1-10 | 0.1485 |
| 12 | Ag ₂ S-PAN | PAN | PNNL | Polymer | Ag, S | Bead | 1-3 | 0.2626 |

2 X-Ray Diffraction Data

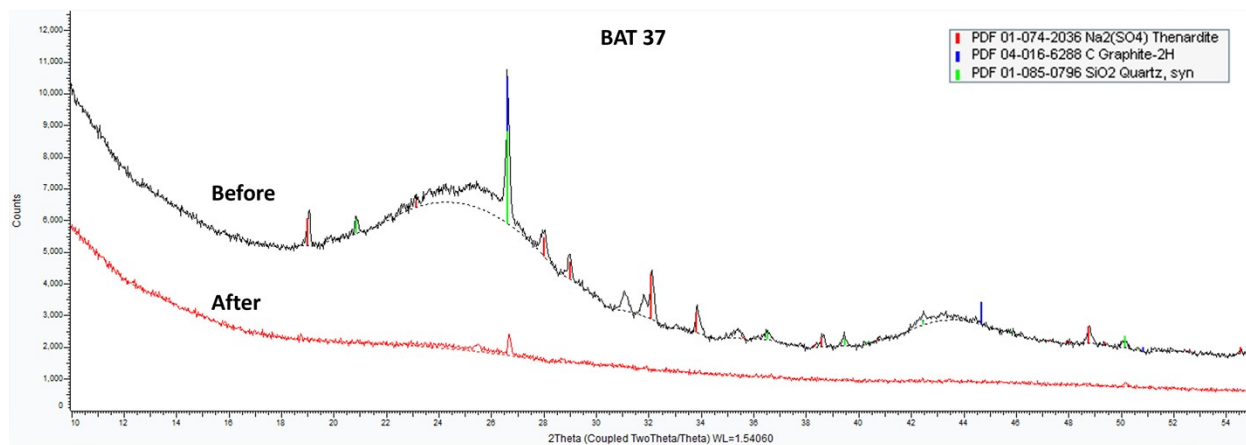


Figure S1. XRD patterns of BAT37 before and after iodine uptake.

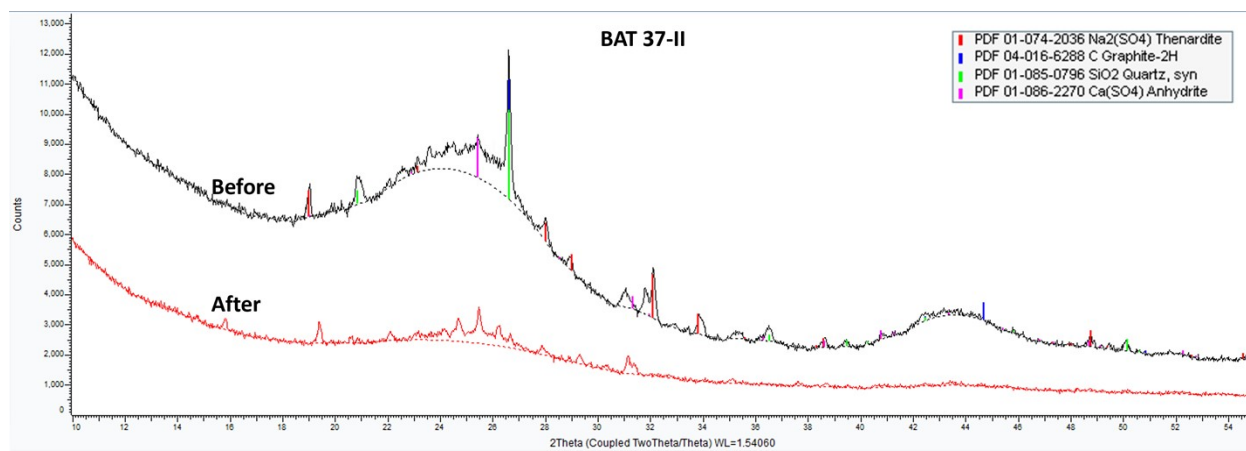


Figure S2. XRD patterns of BAT37-II before and after iodine uptake.

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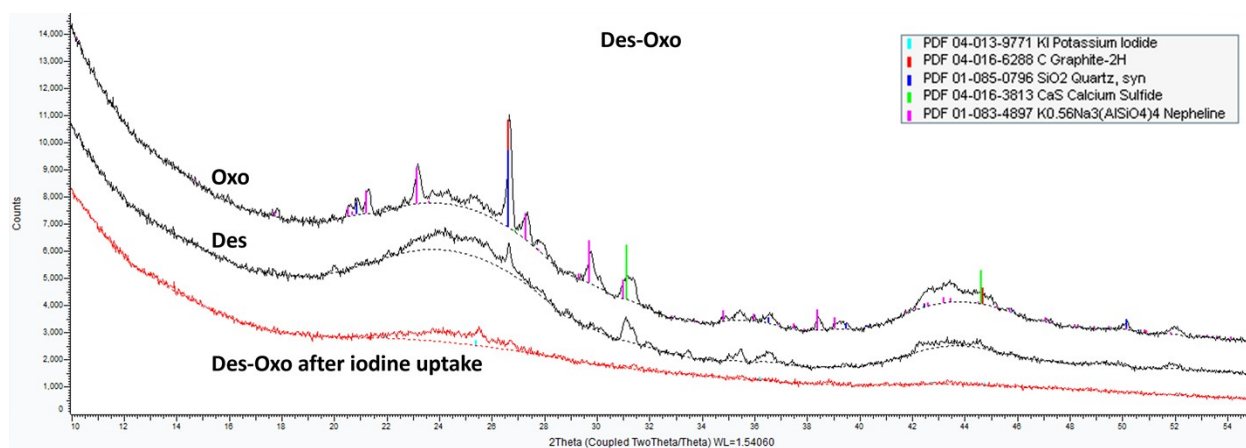


Figure S3. XRD patterns of raw Oxo and Des sorbents before iodine uptake (black) and mixed Des-Oxo sorbent (red) after iodine uptake.

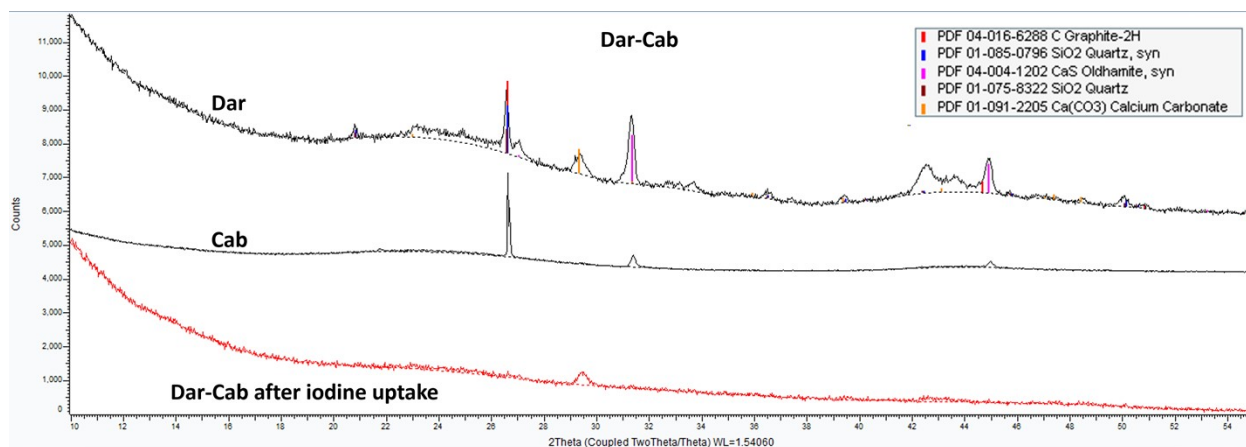


Figure S4. XRD patterns of raw Dar and Cab sorbents before iodine uptake (black) and mixed Dar-Cab sorbent (red) after iodine uptake.

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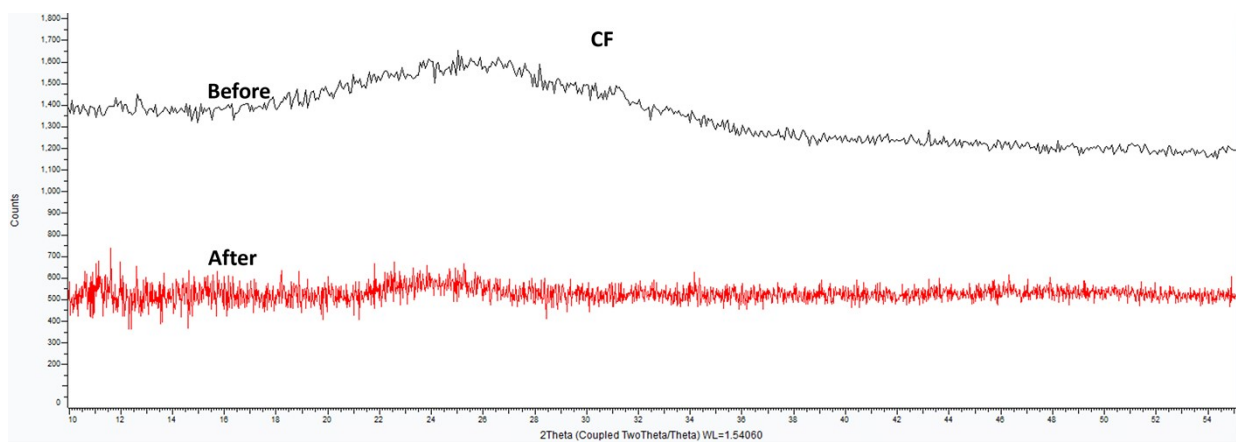


Figure S5. XRD patterns of CF before and after iodine uptake.

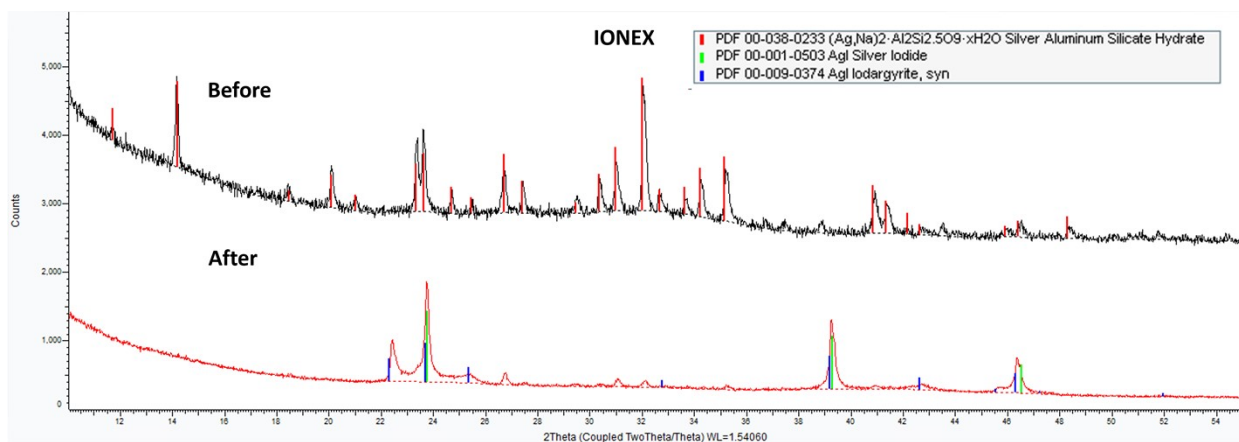


Figure S6. XRD patterns of IONEX before and after iodine uptake.

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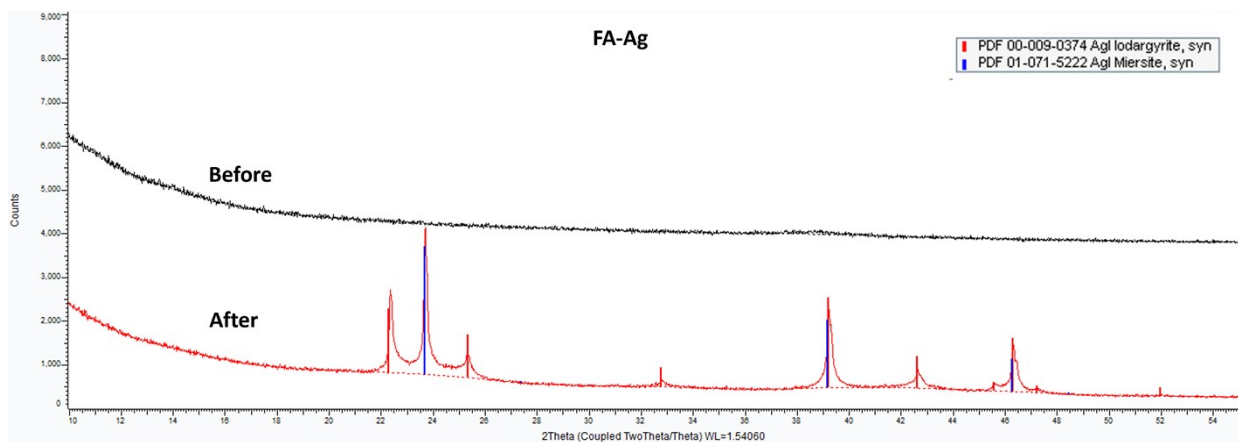


Figure S7. XRD patterns of FA-Ag before and after iodine uptake.

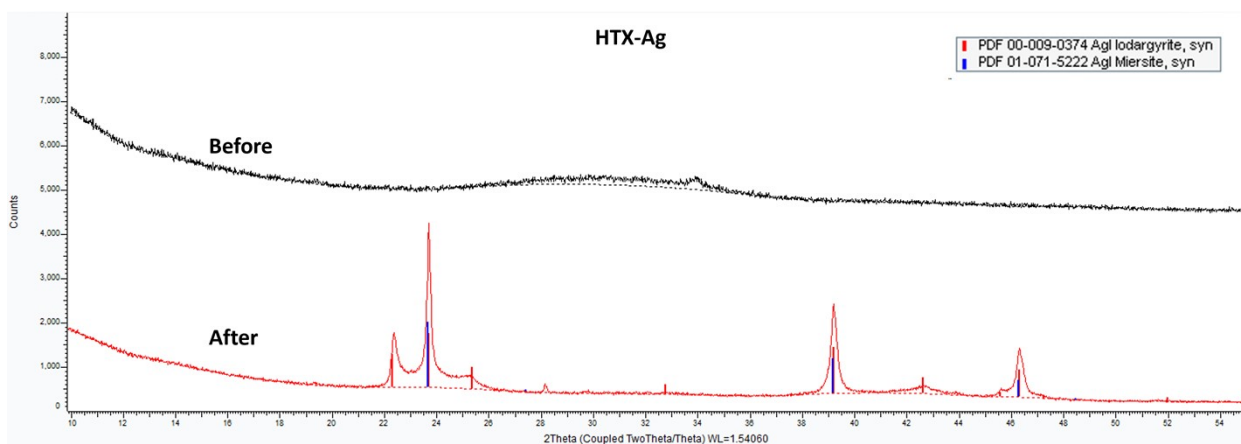


Figure S8. XRD patterns of HTX-Ag before and after iodine uptake.

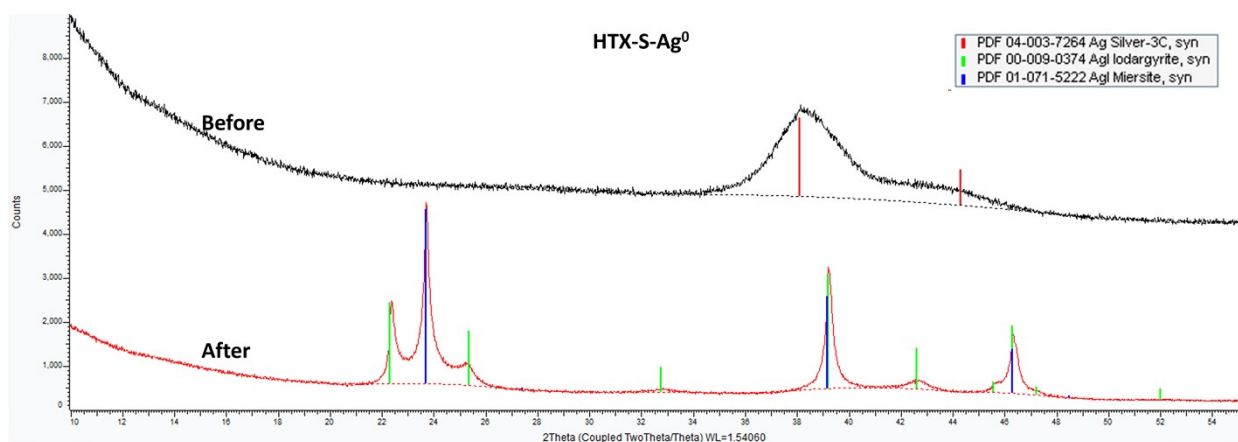


Figure S9. XRD patterns of HTX-S-Ag⁰ before and after iodine uptake.

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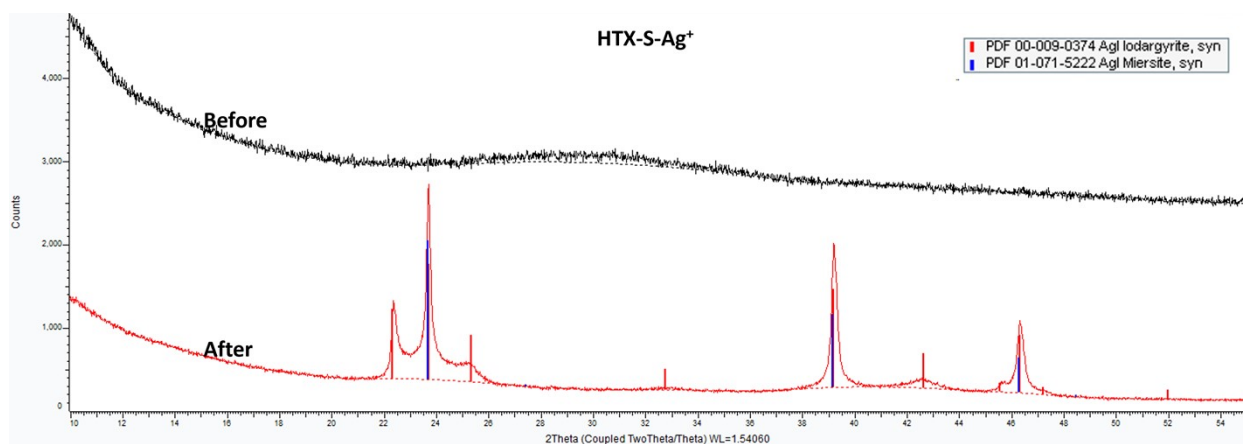


Figure S10. XRD patterns of HTX-S-Ag⁺ before and after iodine uptake.

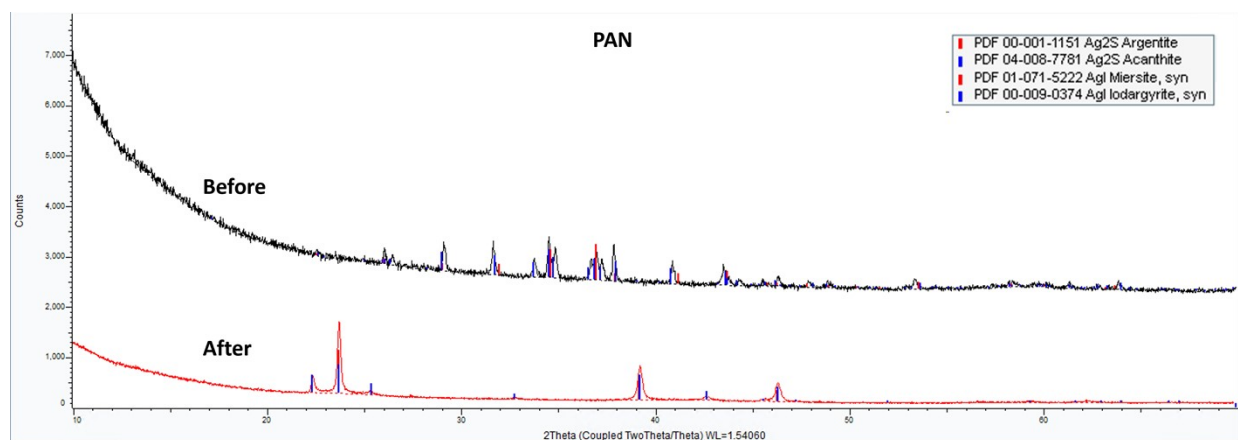


Figure S11. XRD patterns of Ag₂S-PAN before and after iodine uptake.

3 Comparison of IONEX Ag-400 and FA-Ag

In a separate set of loading experiments run after this main set, IONEX Ag-400 was run in triplicate by itself at 150°C and similar values (low variability) were obtained at $q_{e,des} = 292 \pm 7$ mg/g. The goal of these tests was to assess the reproducibility of the static iodine tests and to see if FA-Ag was causing issues during iodine loading tests. Thus, the test details of these experiments are summarized in Table S2 where loading times, desorption times, and loading temperatures were different.

Table S2. Summary of comparison tests run for only IONEX Ag-400 and FA-Ag samples.

| Exp.# | Sorbents | T (°C) | Loading t (days) | Desorption t (days) |
|--------|--------------|----------|--------------------|-----------------------|
| Test-1 | All sorbents | 71±2 | 56 d | 4.7 d |
| Test-2 | IONEX, FA-Ag | 71±2 | 23 d | 1 d |
| Test-3 | IONEX, FA-Ag | 150±4 | 1 d | 1 d |
| Test-4 | IONEX, FA-Ag | 150±4 | 1 d | 1 d |
| Test-5 | IONEX, FA-Ag | 150±4 | 1 d | 1 d |
| Test-6 | IONEX, FA-Ag | 150±4 | 1 d | 1 d |
| Test-7 | IONEX | 150±4 | 1 d | 1 d |

The results are summarized in Figure S12 and show the variability between results for these two samples (i.e., IONEX Ag-400 and FA-Ag) when the conditions are changed. The performance of IONEX Ag-400 was drastically improved when the experiment was run in the presence of FA-Ag, but the performance of FA-Ag was reduced significantly between the desorption step (i.e., $q_{e,max} \rightarrow q_{e,des}$) with Δm_{des} ranging from moderate (i.e., 18.3%, Test-1) to extremely high (i.e., >57% in Test-3 – Test-7). These data show the differences in the performances of sorbents in the presence of different materials where they can interact with each other.

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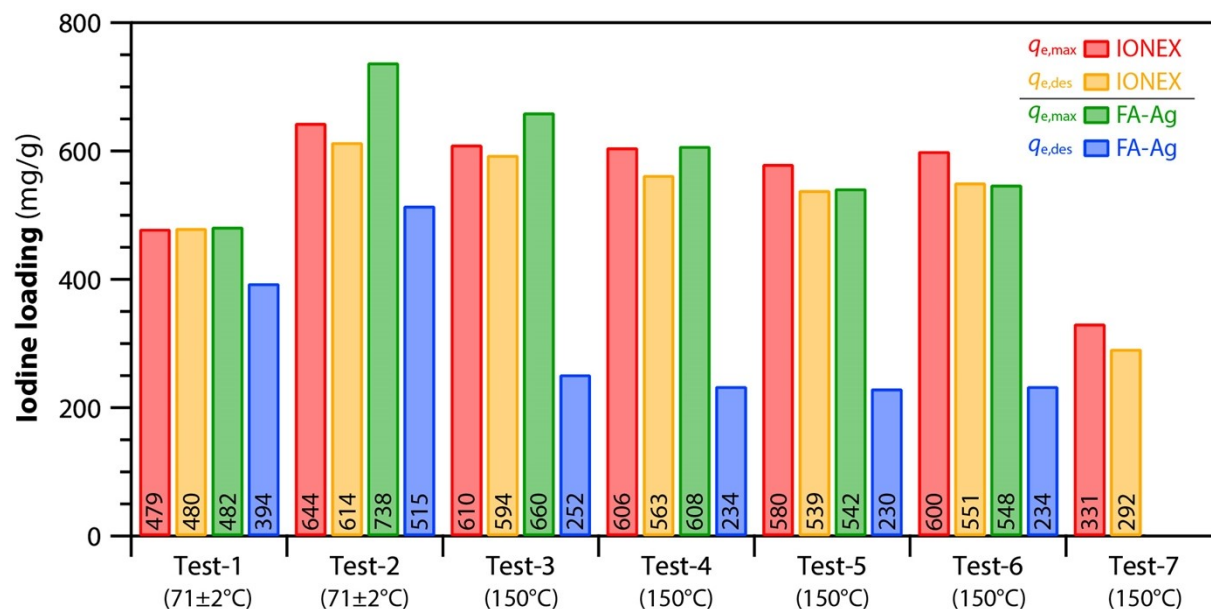


Figure S12. Summary of iodine loading tests for IONEX Ag-400 and FA-Ag including the tests run with the full sample set (Test-1) as well as additional tests run with only these two samples at 71°C (Test-2) and 150°C (Test-3 – Test-6), and an experiment run at 150°C with only IONEX (Test-7). The iodine loading values are provided for each bar at the bottom of the chart.

4 Adsorption Kinetic Model

Table S3. Parameters for the kinetic model

| Samples | 1/k (h) | q_e (mg/g) |
|-----------------------|---------|--------------|
| HTX-S-Ag ⁰ | 43.560 | 584.372 |
| HTX-S-Ag ⁺ | 48.249 | 526.599 |
| PAN | 168.228 | 741.813 |