Supplementary Information (SI) for Nanoscale.

Supporting Information

of

Retarding anion exchanges in lead halide perovskite nanocrystals by ligand immobilization

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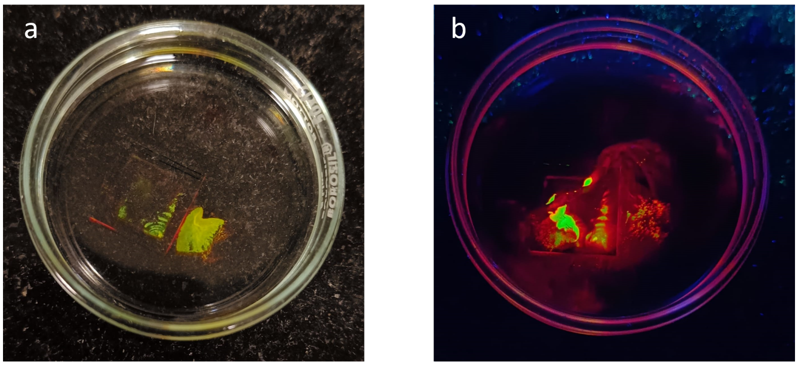

Figure S1. $CsPbBr_3$ NCs film with 20 seconds plasma treatment dipped in PbI_2 solution under (a) ambient light. (b) UV light (365 nm). $CsPbBr_3$ PNCs were comes off from the substrate after dipping in PbI_2 solution.

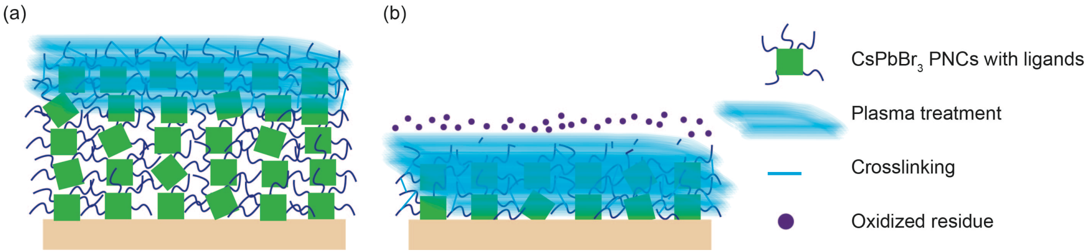

Figure S2: Effect of plasma treatment on $CsPbBr_3$ PNC thin films with various thicknesses - (a) for a thicker film plasma treatment can affect only up to a few layers (b) for a thinner film, plasma treatment can affect the entire film across the depth, leaving the oxidized residues on the surface.

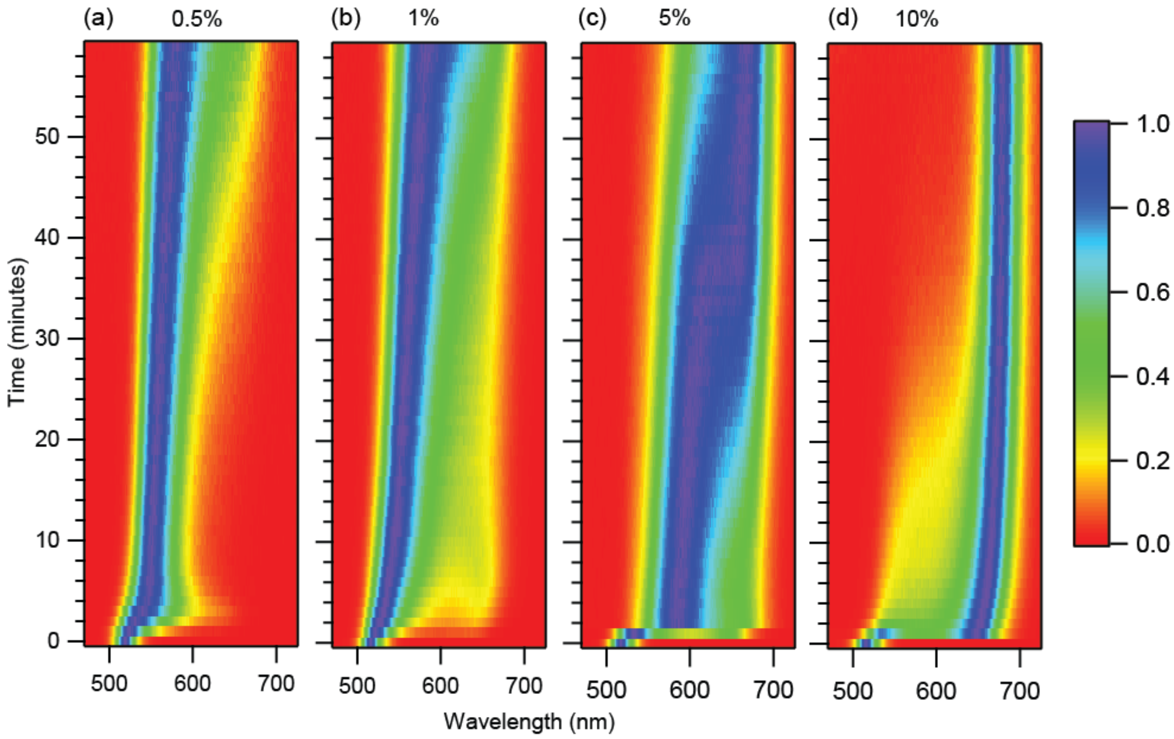

Figure S3: Surface plots for in situ, PL spectra recorded over a 60-minute duration for (a) 0.5%, (b) 1%, (c) 5%, and (d) 10% KI concentration. It shows that with the increase in KI concentration, the rate of anion exchange increases.

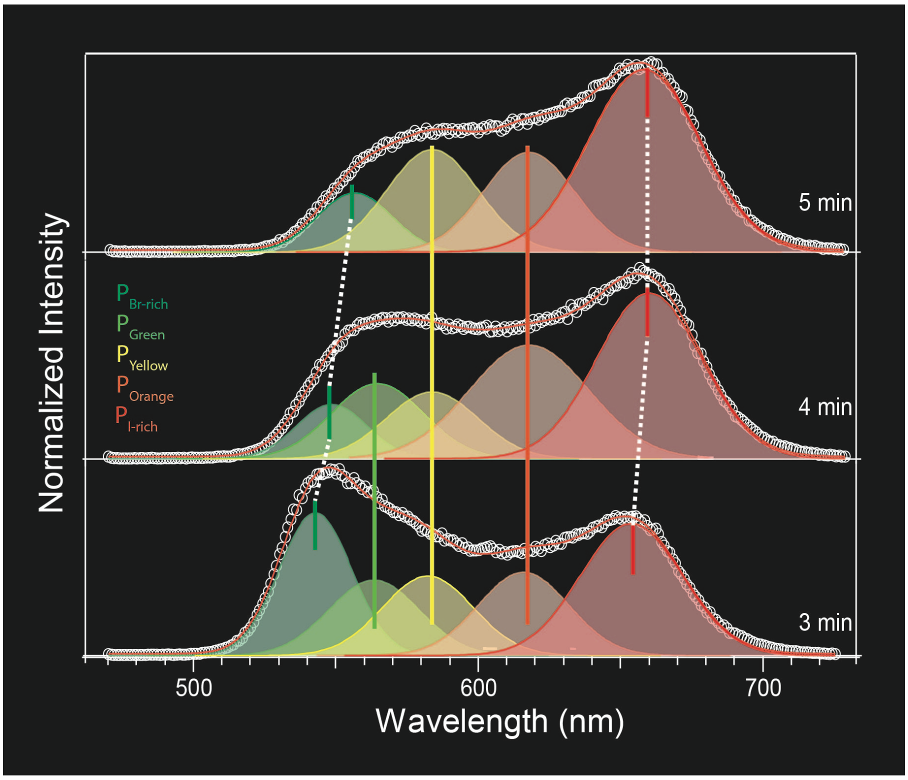

Figure S4. Decomposition of PL spectra for samples without plasma treatment after 3, 5, and 10 minutes of anion exchange. The solid lines indicate that the positions of the intermediate peaks P_{Green}, P_{Yellow}, and P_{Orange} were kept the same, while the $P_{Br\text{-}rich}$ and $P_{I\text{-}rich}$ peak positions were varied up to 4 minutes. After 4 minutes, the $P_{Br\text{-}rich}$ overlapped significantly with P_{Green} and we removed the same during the decomposition, while the P_{yellow} and P_{orange} peaks remained fixed. This fitting method was applied consistently throughout the remaining data analysis.

The extent of mixed halide compositions may vary within the ensemble of the nanocrystals, which is reflected in their broad PL peaks observed during the anion exchange. Since the intermediate compositions cannot be separated, we kept the full width at half maximum (FWHM) and the peak position of the intermediate compositions constant during the decomposition of the PL spectra (i.e., P_{Green}, P_{Yellow}, and P_{Orange} in the following figure). Only the FWHM and peak position of the end peaks on both sides (i.e., $P_{Br\text{-}rich}$ and $P_{I\text{-}rich}$) were allowed to vary. We have observed a systematic shift in these two peak positions. Once the Br-rich significantly overlaps with the intermediate peak, we have not considered the intermediate peak in the decomposition. For example, in the following data, the $P_{Br\text{-}rich}$ peak overlaps significantly with the P_{Green} after 5 minutes of the anion exchange, and we have not considered the P_{Green} peak for decomposition. This approach allowed us to track the evolution of the Br-rich and I-rich peaks more effectively throughout the anion exchange process.

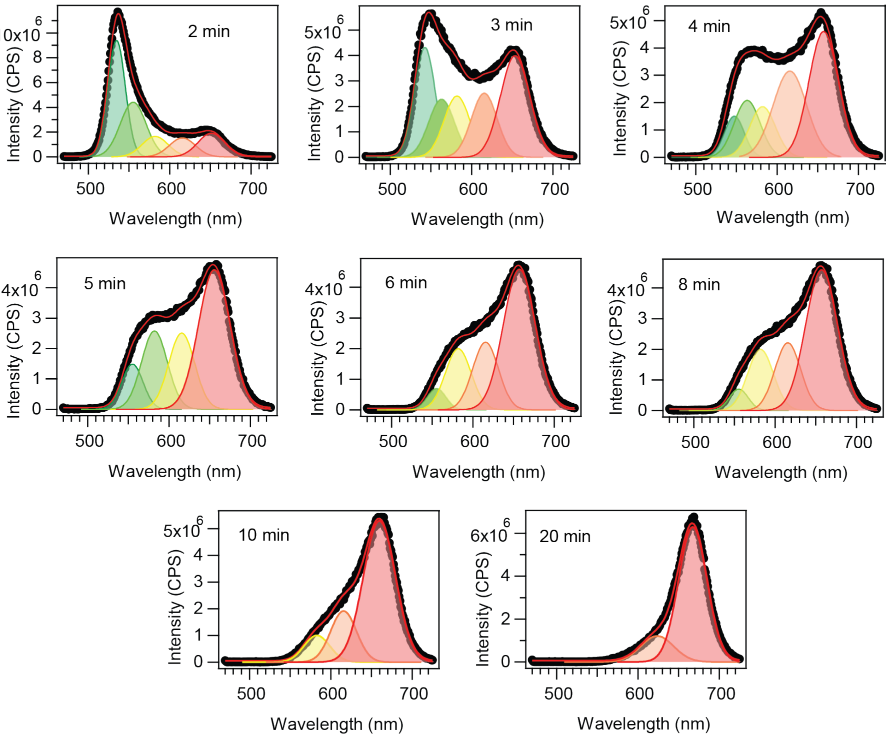

Figure S5a. Decomposition in-situ PL spectra of anion exchange process for no plasma treatment.

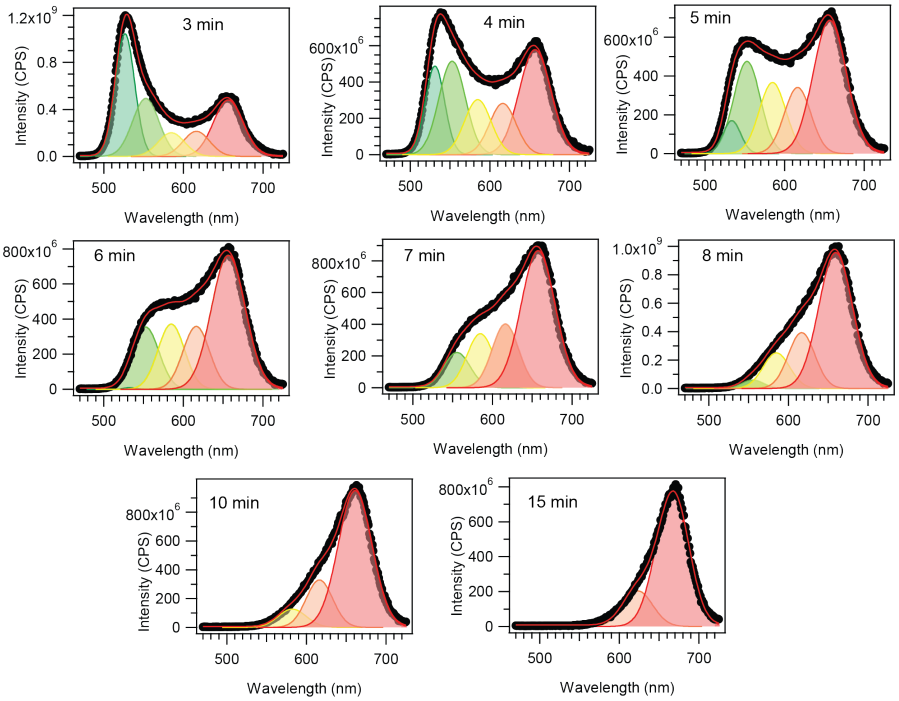

Figure S5b. Decomposition in-situ PL spectra of anion exchange process for 30 seconds plasma treatment.

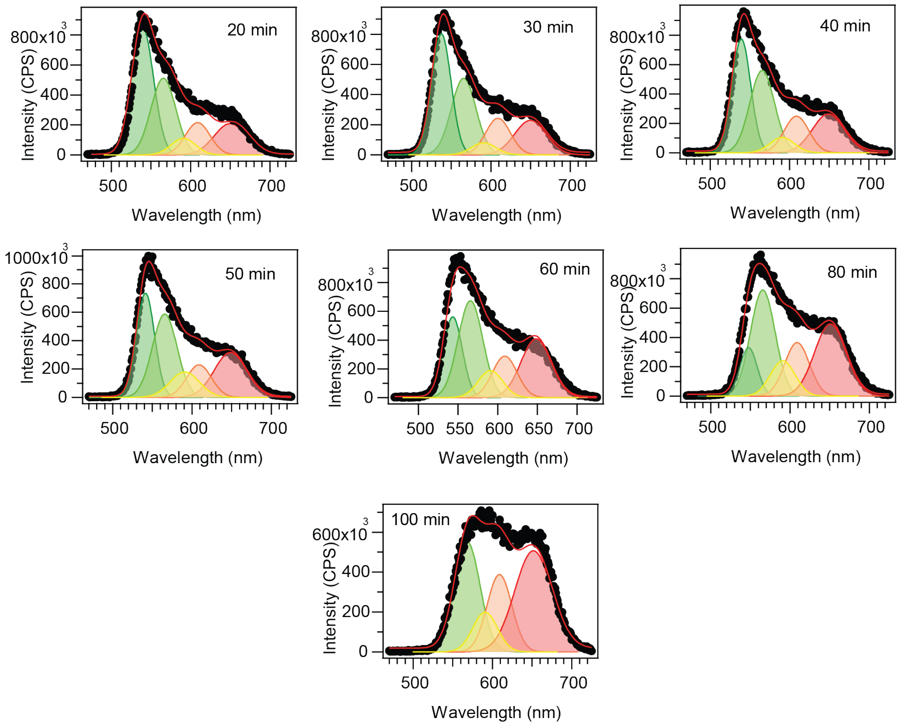

Figure S5c. Decomposition in-situ PL spectra of anion exchange process for 1 minute plasma treatment.

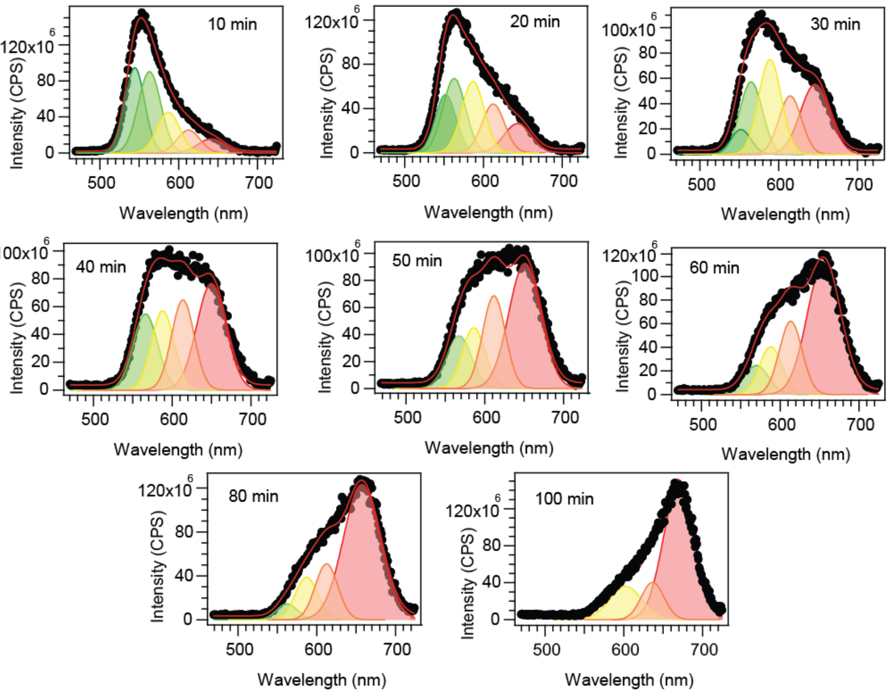

Figure S5d. Decomposition in-situ PL spectra of anion exchange process for 10 minutes plasma treatment and 0.5% KI concentration.

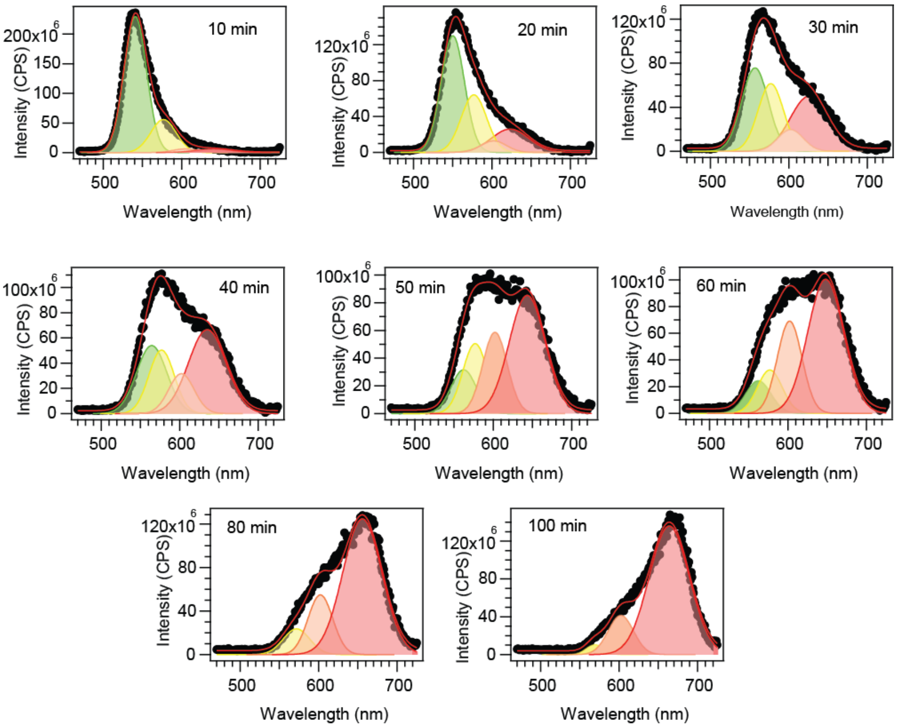

Figure S5e. Decomposition in-situ PL spectra of anion exchange process for 30 minutes plasma treatment.

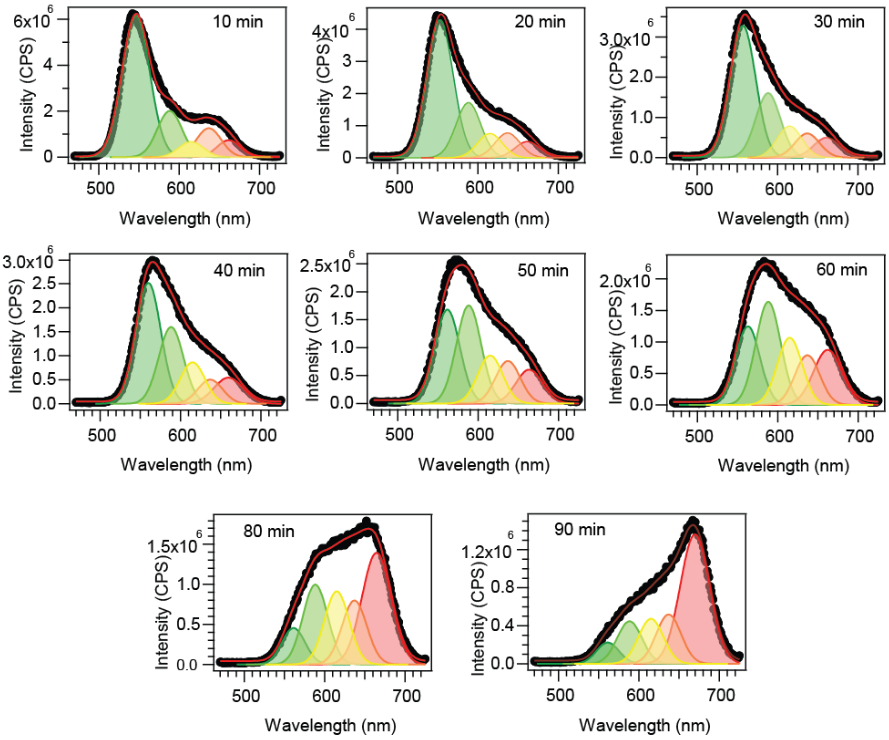

Figure S5f. Decomposition in-situ PL spectra of anion exchange process for 1% KI concentration.

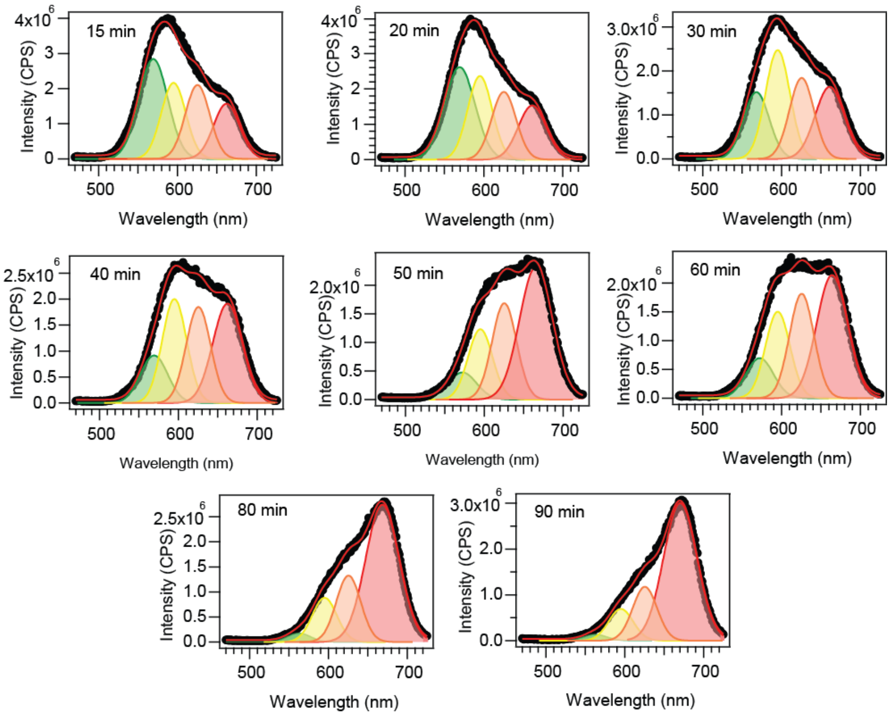

Figure S5g. Decomposition in-situ PL spectra of anion exchange process for 5% KI solution.

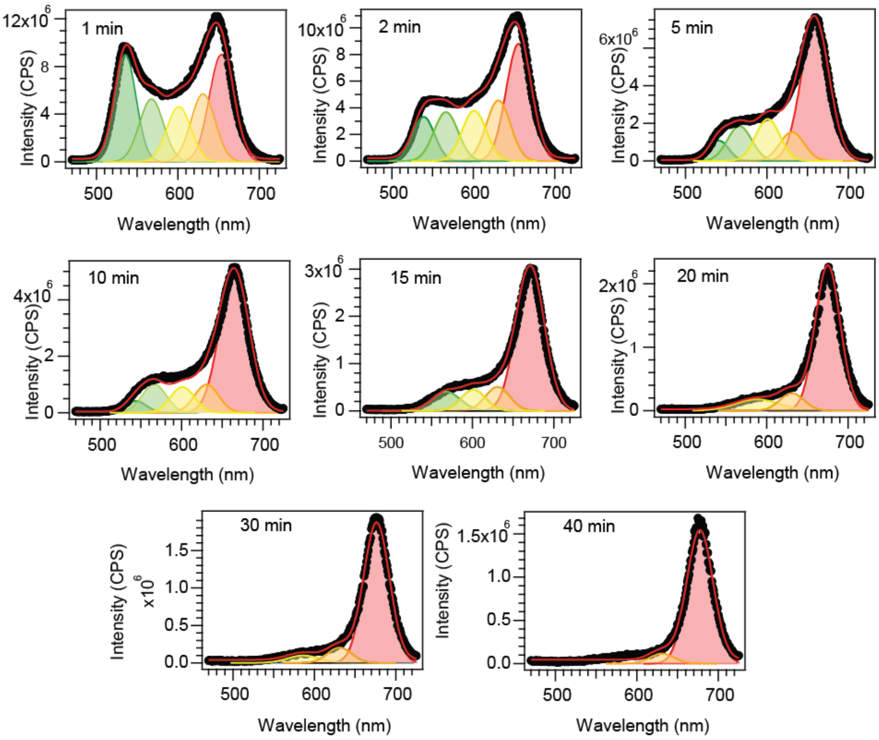

Figure S5h. Decomposition in-situ PL spectra of anion exchange process for 10 % KI concentration.

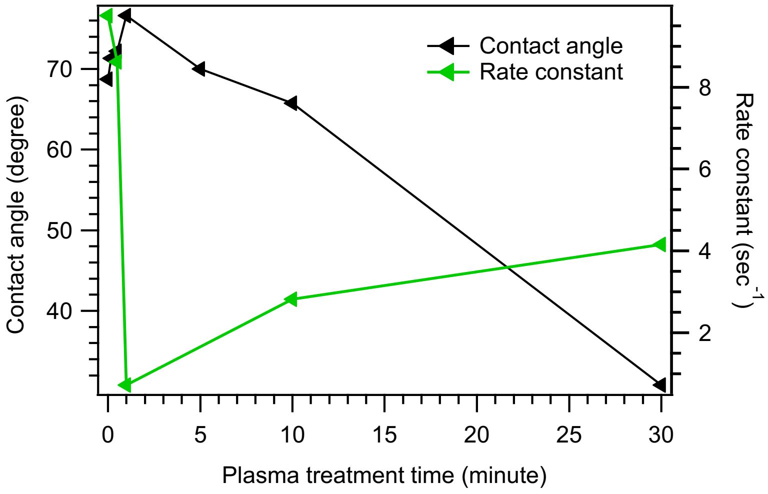

Figure S6: Comparison between water contact angles and anion exchange reaction rates with different plasma treatment times.