Supplementary Information

Automated microfluidic screening of ligand interactions during the synthesis of cesium lead bromide nanocrystals

Shangkun Li,^a Robert W. Baker,^b Ioannis Lignos,^a Zhibo Yang,^a Stavros Stavrakis,^a Philip D. Howes^{*a} and Andrew J. deMello^{*a}

 [1] Institute for Chemical and Bioengineering, Department of Chemistry and Applied Biosciences, ETH Zürich, Vladimir Prelog Weg 1, 8093 Zürich, Switzerland.
[2] Department of Chemistry, University of Bath, Claverton Down, Bath, UK



Figure S1. The entire data set gathered across the four experiments, with the four different ligands sets. These are included to present the raw data prior to data analysis.



Figure S2. The entire data set presented as contour plots, derived from the raw data shown in Figure S1. Note that the colour bar scales differ between the peak position and median emission contour plots.



Figure S3. Positions of the optimal parameters in each experiment in the search for quantumconfined emission (<525 nm), with a balance between maximizing peak intensity and minimizing emission width. The experiments are (a) C8B-C8A, (b) C8Bb-C8A, (c) C8B-CAb, and (d) C8Bb-C8Ab.



Figure S4. (a) TEM micrographs of nine samples taken from the C8Bb-C8A experiment. Scale bar = 100 nm. (b,c) Contour maps of the sampling points in the median emission and interquartile range contour plots. (d) The emission spectra associated with the nine samples marked.

C8B-C8Ab Ligand Set



Figure S5. Screening results for the ligand set C8B-C8Ab. The contour plots show (a) median emission, (b) interquartile range and (c) peak intensity as a function of base:acid ratio and temperature. The white dashed lines in the contour plots correspond to the four spectral series shown in panels (d–g).



Figure S6. (a) TEM micrographs of nine samples taken from the C8B-C8Ab experiment. Scale bar = 100 nm. (b,c) Contour maps of the sampling points in the median emission and interquartile range contour plots. (d) The emission spectra associated with the nine samples marked.





Figure S7. Screening results for the ligand set C8Bb-C8Ab. The contour plots show (a) median emission, (b) interquartile range and (c) peak intensity as a function of base:acid ratio and temperature. The white dashed lines in the contour plots correspond to the four spectral series shown in panels (d–g).



Figure S8. (a) TEM micrographs of nine samples taken from the C8Bb-C8Ab experiment. Scale bar = 100 nm. (b,c) Contour maps of the sampling points in the median emission and interquartile range contour plots. (d) The emission spectra associated with the nine samples marked.