Electronic Supplementary Information (ESI) for

Probing Organic Ligands and their Binding Schemes on Nanocrystals by

Mass Spectrometric and FT-IR Spectroscopic Imaging

Jin Gyeong Son, ^{a,b} Eunjin Choi,^{c,d} Yuanzhe Piao,^{c,d} Sang Woo Han, *,^a and Tae Geol Lee*,^b

^aDepartment of Chemistry and KI for the NanoCentury, KAIST, Daejeon 34141, Korea

^bCenter for Nano-Bio Measurement, Korea Research Institute of Standard and Science, Daejeon 34113, Korea

^cProgram in Nano Science and Technology, Department of Transdisciplinary Studies, Graduate School of

Convergence Science and Technology, Seoul National University, Seoul 08826, Korea

^dAdvanced Institute of Convergence Technology, Suwon 16227, Korea

*To whom all correspondence should be addressed.

Tel: +82-42-350-2812; Fax: +82-42-350-2810 *E-mail : sangwoohan@kaist.ac.kr* (SWH)

Tel: +82-42-868-5129; Fax: +82-42-868-5032 *E-mail : tglee@kriss.re.kr* (TGL)



Fig. S1 (a) TEM image and (b) UV-vis absorption and PL spectra of CdSe/ZnS QDs.



Fig. S2 Comparison of ToF-SIMS data obtained from CdSe/ZnS QDs (a) before and (b) after purification at negative ion mode. Scale bars indicate 50 μm.



Fig. S3 TOF-SIMS spectra of ions presented in Fig. 1 and S2 in the ESI. Upper and lower traces are obtained before and after the purification, respectively.



Fig. S4 IR spectra of free ligands in hexane. The peak intensities in the right column were doubled as compared to the left column.



Fig. S5 XPS spectra for the P 2p core level of the sample before and after the purification. XPS measurements were carried out using a Thermo VG Scientific Sigma Probe spectrometer using Al K α X-ray (1486.6 eV) as the light source. XPS data were calibrated using the C 1s peak at 285.0 eV. As shown the above figure, alkyl phosphine (131.4 eV) and alkyl phosphonate (132.5 eV) species were prevalent in the sample before and after the purification, respectively (refs. 20 and 22 in text).