Supplementary Materials

Cd_3P_2/Zn_3P_2 Core-Shell Nanocrystals: Synthesis and Optical Properties

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Figure S1: Low (left) and high (right) resolution transmission electron microscopy images of Cd_3P_2 cores synthesized with hexadecylamine as the surfactant.

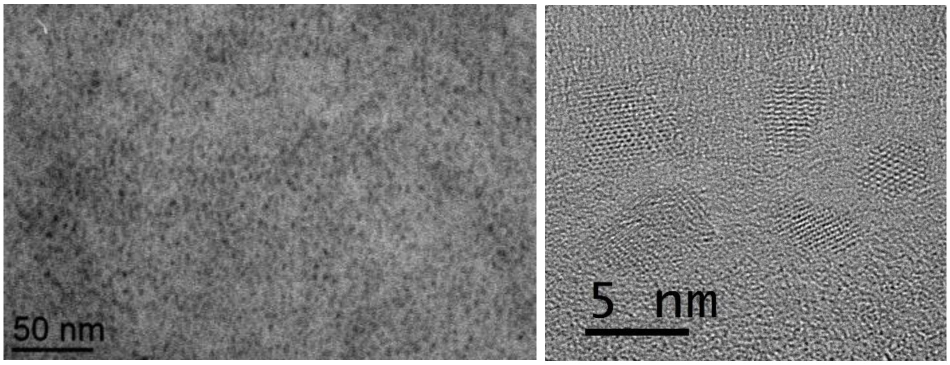


Figure S2: High resolution transmission electron microscopy of Cd_3P_2/Zn_3P_2 nanocrystals and XRD patterns of Cd_3P_2 cores (blue), Cd_3P_2/ Zn_3P_2 (red), the relevant reflections are highlighted for Cd_3P_2 00-002-1182 and Zn_3P_2 01-002-1264. The * symbol denotes reflections that are caused by the kapton film.

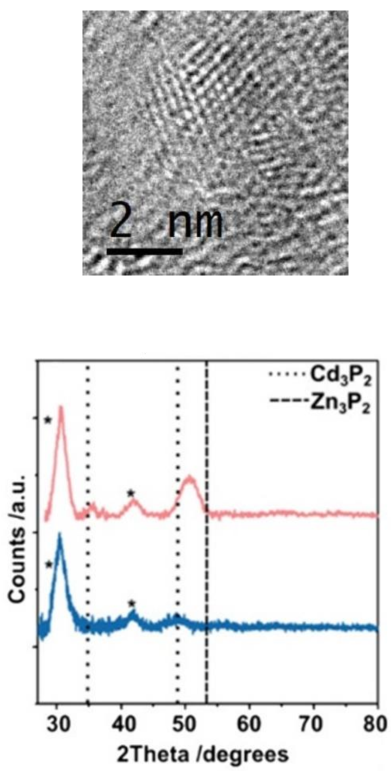


Table S1: Composition of synthesized nanocrystals from ICP-MS, EDX, and XPS measurements. XPS compositions were determined from the P 2p, Zn 3s and Cd 3d core peaks.

Sample	ICP-MS	EDX	XPS
Cd_3P_2	**0.119 mmol Cd; 0.081 mmol P ($Cd_{2,94}P_2$)**	**64 % Cd; 36 % P ($Cd_{3.55}P_2$)**	**$Cd_{3.2}P_2$**
Cd_3P_2/Zn_3P_2	**0.111 mmol Cd; 0.322 mmol Zn; 0.273 mmol P ($Cd_{0,81}Zn_{2,36}P_2$) With a $Cd_{2.94}P_2$ core, shell composition is found to be $Zn_{3.26}P_2$**	**18 % Cd; 45 % Zn; 37 % P ($Cd_{0,97}Zn_{2,43}P_2$) With a $Cd_{3.55}P_2$ core, shell composition is found to be $Zn_{3,35}P_2$**	**$Cd_{1,1}Zn_{2,2}P_2$ With a $Cd_{3.2}P_2$ core, shell composition is found to be $Zn_{3,3}P_2$**

Table S2: XRD peak maxima and Full Width at Half Maxima for the (220) plan of Cd_3P_2 and Cd_3P_2/Zn_3P_2

Sample	Peak maxima (°)	Peak FWHM (°)
Cd_3P_2 cores	**48.8°**	**3.88**
Cd_3P_2/Zn_3P_2	**50.7°**	**2.95**

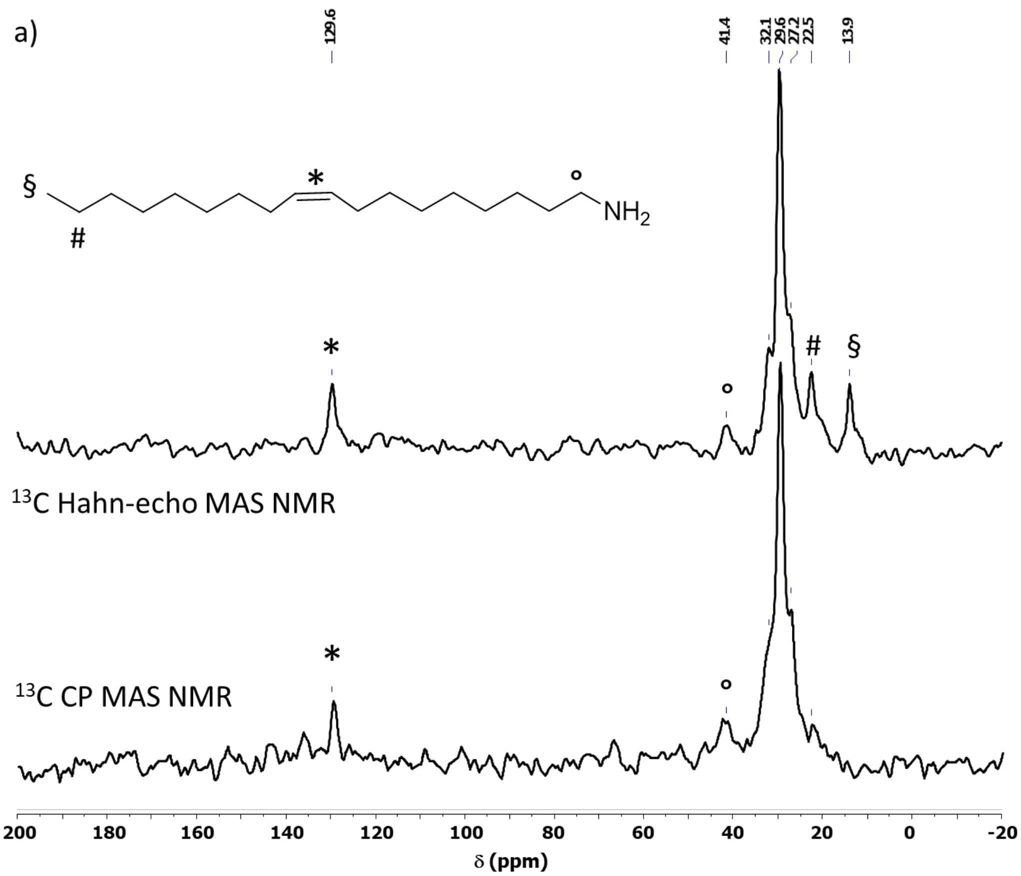
Table S3: Time resolved emission measurements: average emission lifetimes of Cd_3P_2 and Cd_3P_2/Zn_3P_2 core-shell nanocrystals.

Sample	Coeff A1	Average lifetime (t_1)	Coeff A2	Average lifetime (t_2)
Cd_3P_2 cores	**0,75**	**110 ns**	**0,25**	**290 ns**
Cd_3P_2/Zn_3P_2	**0,25**	**140 ns**	**0,75**	**290 ns**

I=A1*exp(-t/t1)+A2*exp(-t/t2)+yo (noise level)

Figure S3: Magic Angle Spinning NMR of Cd_3P_2/Zn_3P_2: 3a) 13C CP MAS NMR spectra of Cd_3P_2/Zn_3P_2, 3b) 31P Hahn-echo MAS NMR spectra of Cd_3P_2/Zn_3P_2.

a)



b)

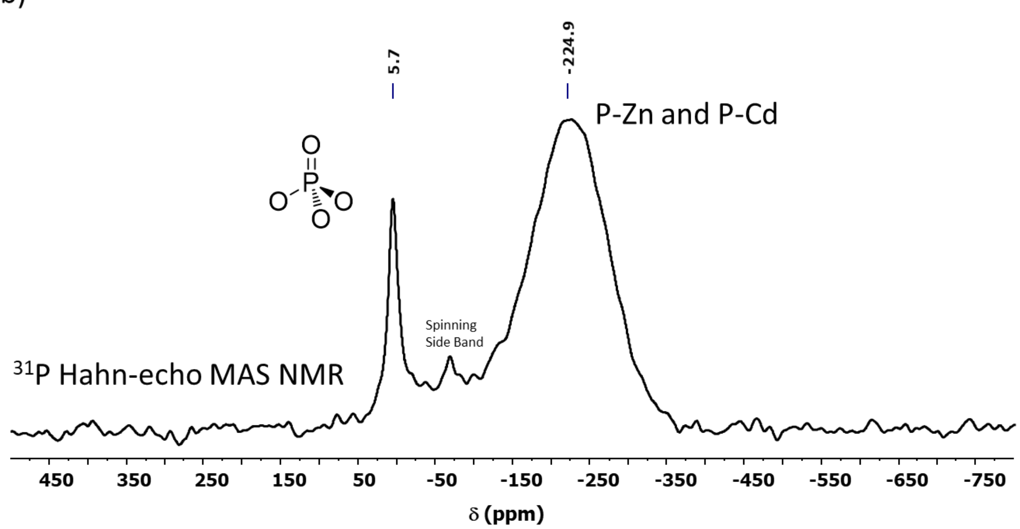


Figure S4: High resolution XPS of Cd_3P_2/Zn_3P_2: a) P 2p and Zn 3s core peaks; b) Cd 3d core peaks, the detection of a N 1s peak at ca. 399.0 eV is due to the presence of Nitrogen atoms in the oleylamine ligands; c) Zn 2p core peaks. The presence of Carbon and Oxygen is also detected through O 1s and C1 core peaks (not shown here).