

Supplementary Information

From (Cd₂Se₂)(pa) (pa = propylamine) hybrid precursors to various CdSe nanostructures: structural evolution and optical properties**

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Crystal structural refinement based on the PXRD:

The powder X-ray diffraction analysis of 2D-[(Cd₂Se₂)(pa)] was performed on a Rigaku D/M-2200T automated diffraction system (Ultima+) with Cu K radiation. Intensities were collected in a 2θ range of 3-55° at room temperature with a step size of 0.05° and a counting time of 2S/step at the operating powder of 40 kV/40 mA. The powder pattern was indexed by TREOR method using program PowderX and the space group was determined to be *Pbca*. An initial structural model were created for the Rietveld profile refinement in GSAS, based on the structure of the double-layered [Zn₂Se₂(ba)] (ba = n-butylamine).¹ The initial refinement of background, unit cell parameters, and several parameters of profile function such as LX, LY, GW, GU, GV were refined one by one. All non hydrogen atoms were refined with fixed thermal parameters. Hydrogen atoms were not added. The details of the Rietveld refinements as well as crystal data of the proposed structure are listed in Table S1

Table S1. GSAS Rietveld Refinement results for 2D-[(Cd₂Se₂)(pa)].

Empirical formula	C ₃ H ₉ NSe ₂ Cd ₂
Fw	432.78
space group	<i>Pbca</i> (No.61)
a(Å)	7.1809(6)
b(Å)	6.8785(2)
c(Å)	36.659(5)
V(Å ³)	1810.7(7)
Z	8
T	293(2)
λ(Å)	1.413
ρ _{calc}	3.17
pattern range(°)	3-55
step size(2θ, °)	0.05
step scan time (s)	2
no. of contributing reflns	672
no. of struc. params	87

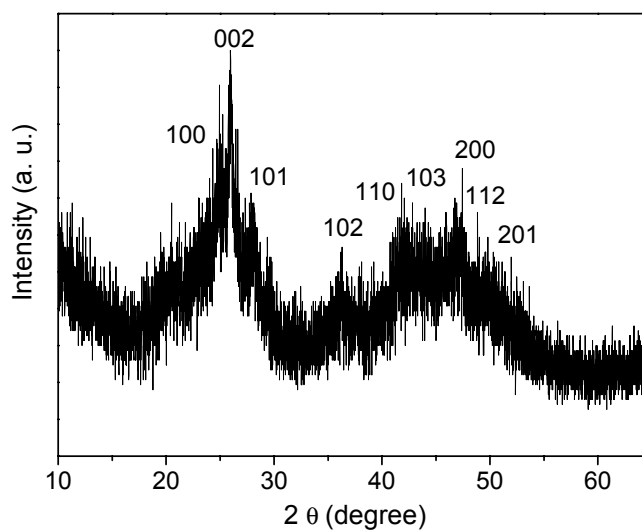


Figure S1. The PXRD pattern of CdSe nanoparticles obtained from (Cd₂Se₂)(pa) pyrolysis at 250 °C under ambient atmosphere. The phase is determined as wurtzite CdSe.