Supporting Information

Structure and Properties of $Cd_4P_2Cl_3$, an Analogue of CdS

Anand Roy[1], U. Sandhya Shenoy[2], K. Manjunath[1], Pratap Vishnoi [1], Umesh V. Waghmare[2] and C. N. R. Rao.[1*]

[1]New Chemistry Unit, International Centre for Materials Science(ICMS) and CSIR Centre of Excellence in Chemistry, Sheikh Saqr Laboratory, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur P.O., Bangalore- 560064, India. [2]Theoretical Sciences Unit Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur P.O., Bangalore- 560064. *To whom correspondence should be addressed (Email: cnrrao@jncasr.ac.in. Phone : 91-80-23653075))

Materials

Cd-powder (99.5 % metal basis), $CdCl_2$ (99.9 % trace metal basis), and $H_2PtCl_6.6H_2O$ (37.5 % metal basis) was purchased from sigma Aldrich, P-red was purchased from spectrochem (97-98 % assay), NH_4Cl (AR grade, 99.5%), $Cd(CH_3COO)_2.2H_2O$ (SD Fine Chem Ltd, India, 99.0 %), $Na_2S.xH_2O$ (SD Fine Chem Ltd, India, 55-60 %), NaOH (SD Fine Chem Ltd, India, 85.5 %), Na_2SO_3 (SD Fine Chem Ltd, India, 97 %), De-ionized water was used for the experiments.

Synthesis

Cd_3P_2 synthesis

In a typical synthesis of pure phase of Cd_3P_2 of Cd-powder and red-P (3:2.5 mole ratio) was ground for 20 min, to make a homogenous mixture. This intimate mixture was transferred in a quartz ampoule which was sealed under vacuum. The sealed ampoule was heated at 400 $^{\circ}$C for 4 hours in a muffle furnace with the ramp rate of 2.5°/min.

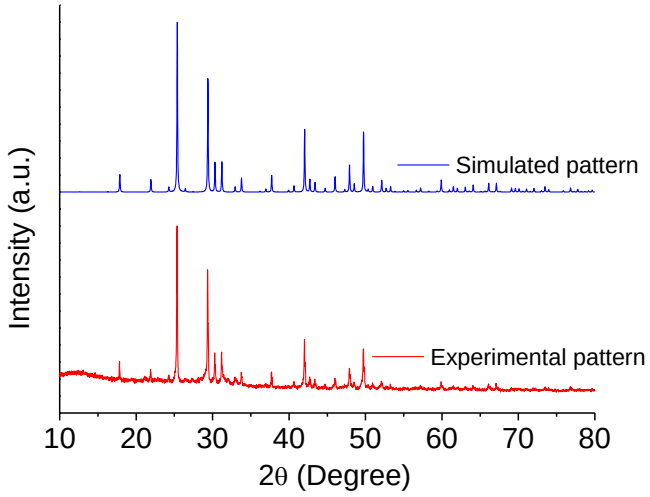

Figure S1: Simulated and experimental PXRD patterns of $Cd_4P_2Cl_3$-1.

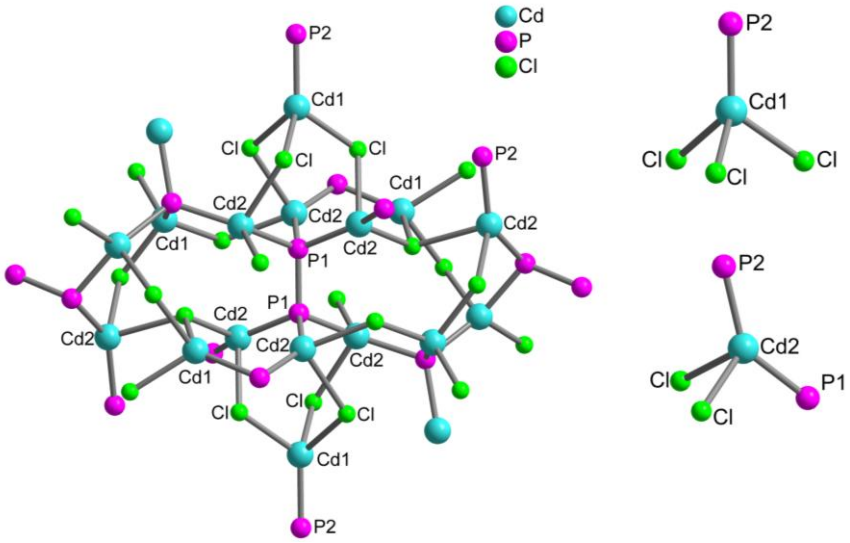

Figure S2. Ball and stick model for the crystal structure of $Cd_4P_2Cl_3$-1, inset shows two different Cd atoms in compound.

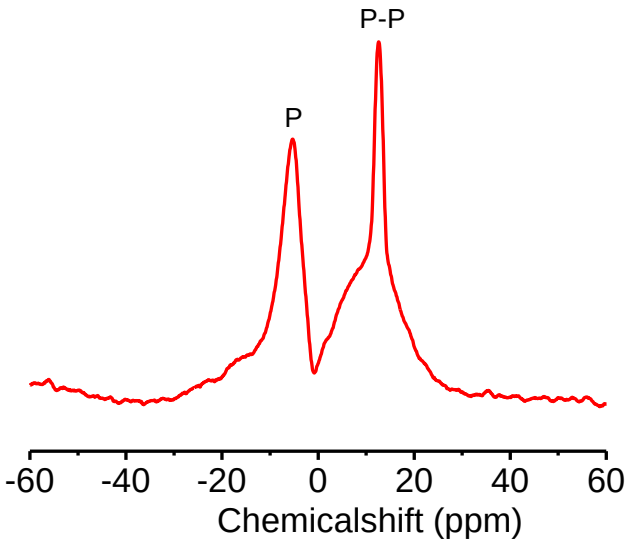

Figure S3. ^{31}P NMR spectra of $Cd_4P_2Cl_3$.

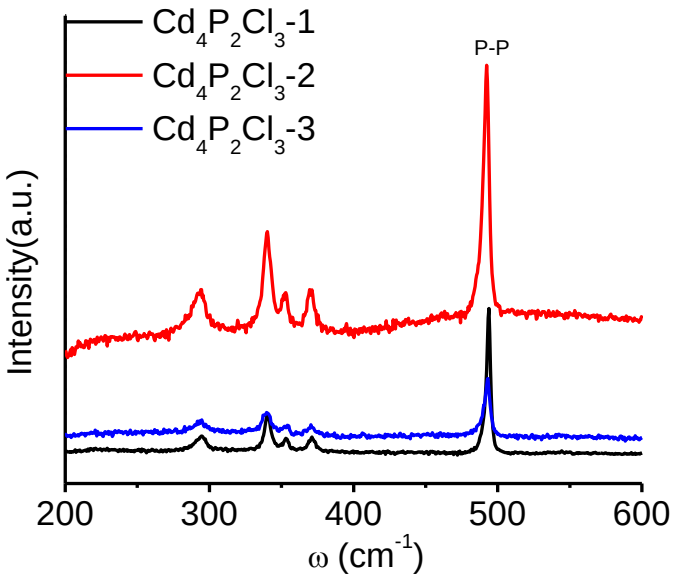

Figure S4. Raman spectra of $Cd_4P_2Cl_3$ compounds prepared by different method.

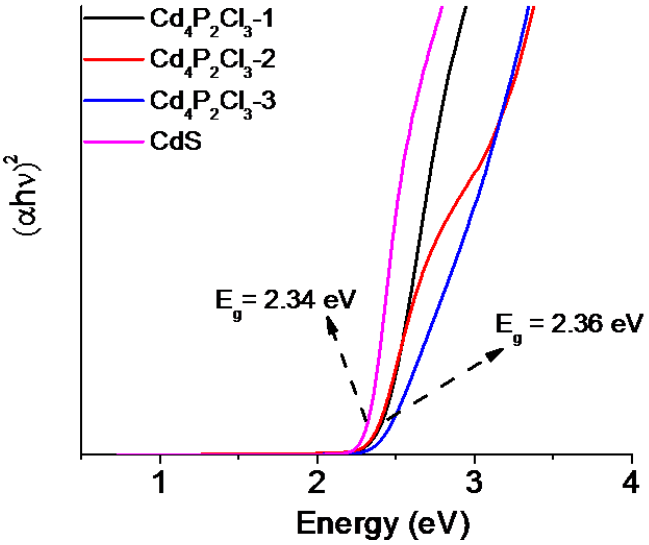

Figure S5. Tauc plots for CdS and $Cd_4P_2Cl_3$ samples.

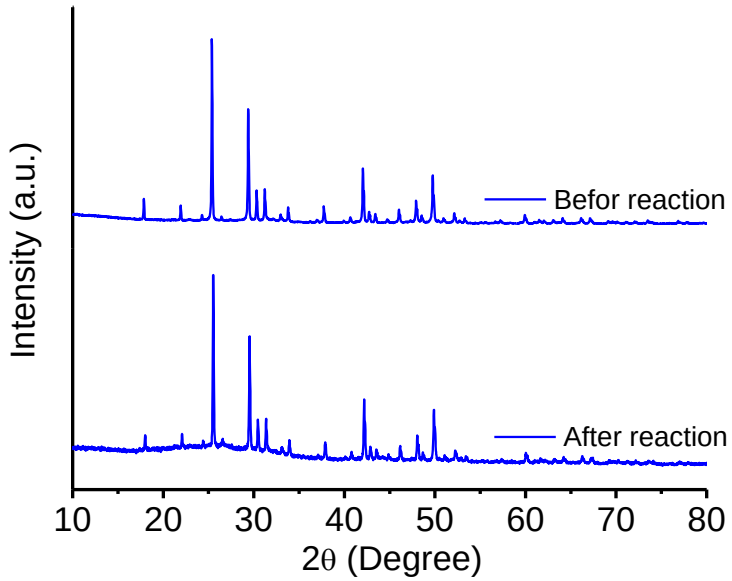

Figure S6. PXRD patterns of $Cd_4P_2Cl_3$-2 before and after photocatalytic reaction.

Table S1.Crystal data and structure refinement for $Cd_4P_2Cl_3$-1.

Empirical formula	$Cd_4Cl_3P_2$
Formula weight	617.89
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Cubic
Space group	*Pa* -3
a	12.1474(7) Å
b	12.1474(7) Å
c	12.1474(7) Å
α	90°
β	90°
γ	90°
Volume	1792.5(3) $Å^3$
Z	8
Density (calculated)	4.579 Mg/m^3
Absorption coefficient	10.521 mm^{-1}
Crystal size	0.300 x 0.150 x 0.100 mm^3
θrange for data collection	2.904 to 24.955°
Reflections collected	2701
R(int)	0.0525
Data / restraints / parameters	529 / 0 / 29
GOF on F^2	0.973
Final R indices [I>2sigma(I)]	R1 = 0.0233, wR2 = 0.0396
R indices (all data)	R1 = 0.0310, wR2 = 0.0409
Largest diff. peak and hole	0.576 and -0.583 $e.Å^{-3}$