

Table SI1 Hydrogen bonding

MCl₂L1 (**1**)

D-H	d(D-H)	d(H···A)	∠DHA	d(D···A)	A
C3-H3	0.930	2.821	139.72	3.581	Cl1 [x+1/2, -y+3/2, z-1/2]
C11-H11A	0.960	2.840	127.49	3.508	Cl1
C11-H11C	0.960	2.769	158.71	3.680	Cl2 [-x+1, -y+1, -z+2]
C12-H12A	0.970	2.637	121.74	3.254	N2
O2-H2	0.820	2.322	168.89	3.130	Cl1 [-x+3/2, y-1/2, -z+3/2]

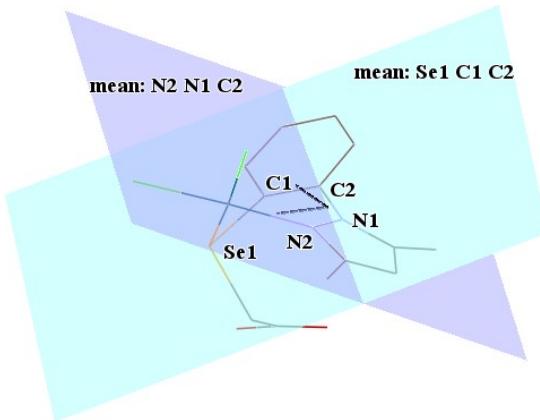
MCl₂L2 (**2**)

D-H	d(D-H)	d(H···A)	∠DHA	d(D···A)	A
C11-H11B	0.960	2.591	147.81	3.441	O2 [-x+1, -y, -z+2]
C11-H11C	0.960	2.911	143.81	3.729	Cl2 [-x, -y, -z+2]
C12-H12A	0.970	2.641	111.21	3.126	N1
C12-H12B	0.970	2.702	134.40	3.451	Cl2 [-x, -y, -z+2]
C13-H13A	0.970	2.907	148.47	3.768	Cl2 [x+1, y, z]
O2-H1O2	0.826	2.291	158.68	3.075	Cl1 [x+1, y-1, z]

MCl₂L3 (**3**)

D-H	d(D-H)	d(H···A)	∠DHA	d(D···A)	A
O1-H1	0.820	2.359	165.79	3.160	Cl1 [x-1, y, z]
C3-H3	0.930	2.715	162.26	3.612	Cl2 [x+1/2, -y+3/2, z-1/2]
C12-H12B	0.970	2.575	120.81	3.183	N2
C12-H12B	0.970	2.588	124.49	3.237	N1
C10-H10A	0.960	2.969	165.05	3.904	Cl1 [x-1/2, -y+3/2, z-1/2]
C10-H10C	0.960	2.952	165.62	3.889	Cl2 [x+1/2, -y+3/2, z-1/2]
C11-H11A	0.960	2.716	137.04	3.481	Cl1

(A)



(B)

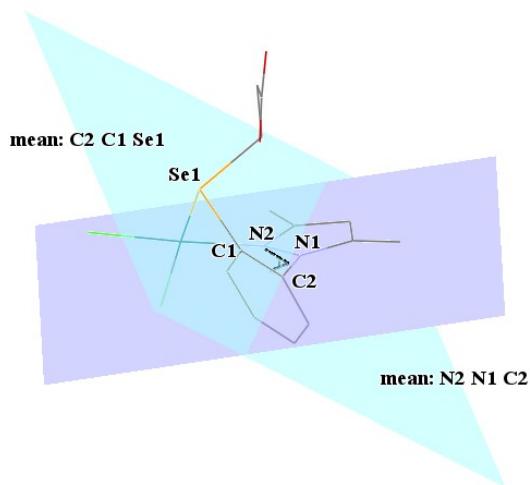


Fig. SI1. (a) Mercury wireframe diagram showing angle formed by intersection of planes Se1C1C2 and N2N1C1 for (a) complex **1** and (b) complex **2**.

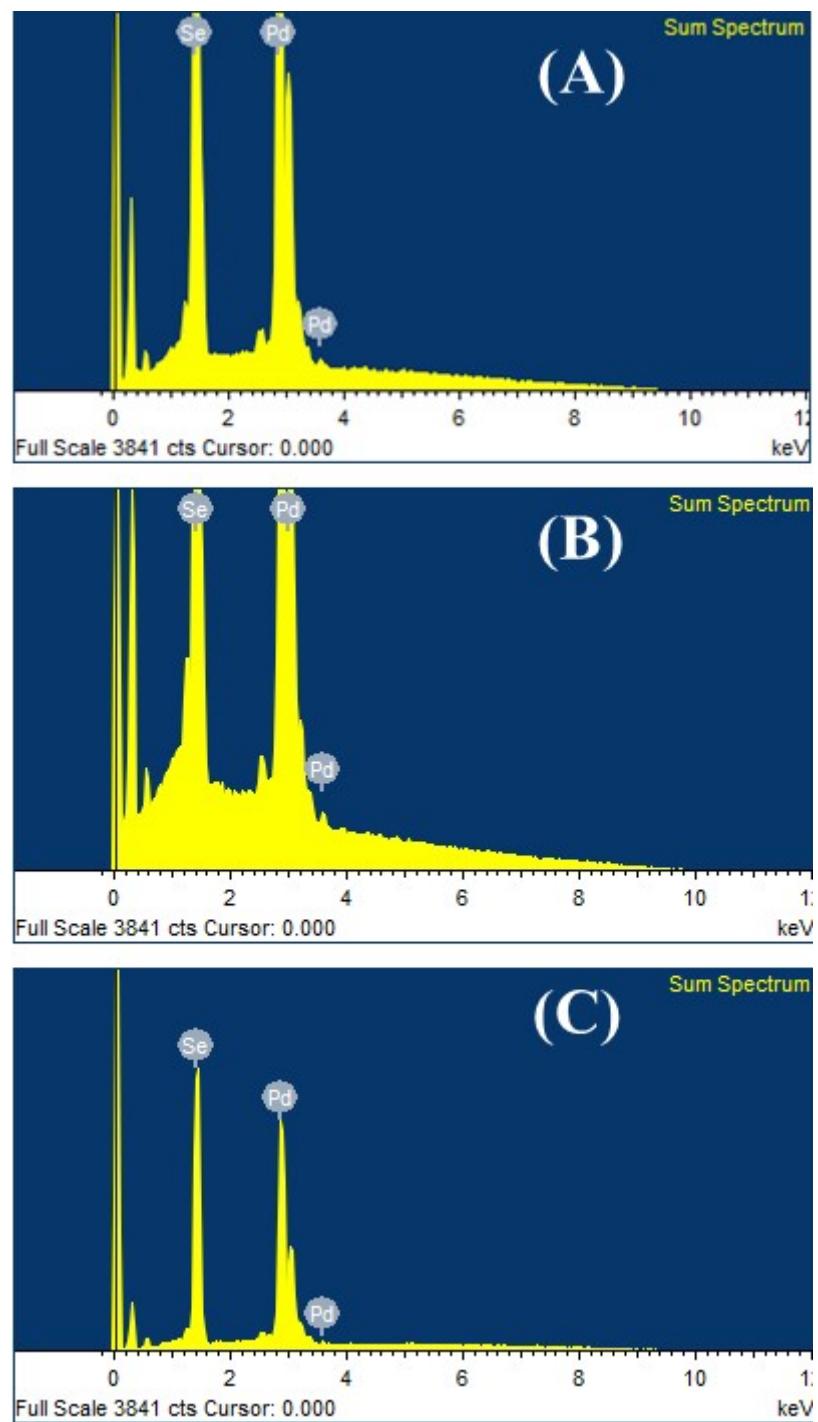


Fig. SI2 EDAX for MSNP obtained from (a) PdL1 (b) PdL2 (c) PdL3

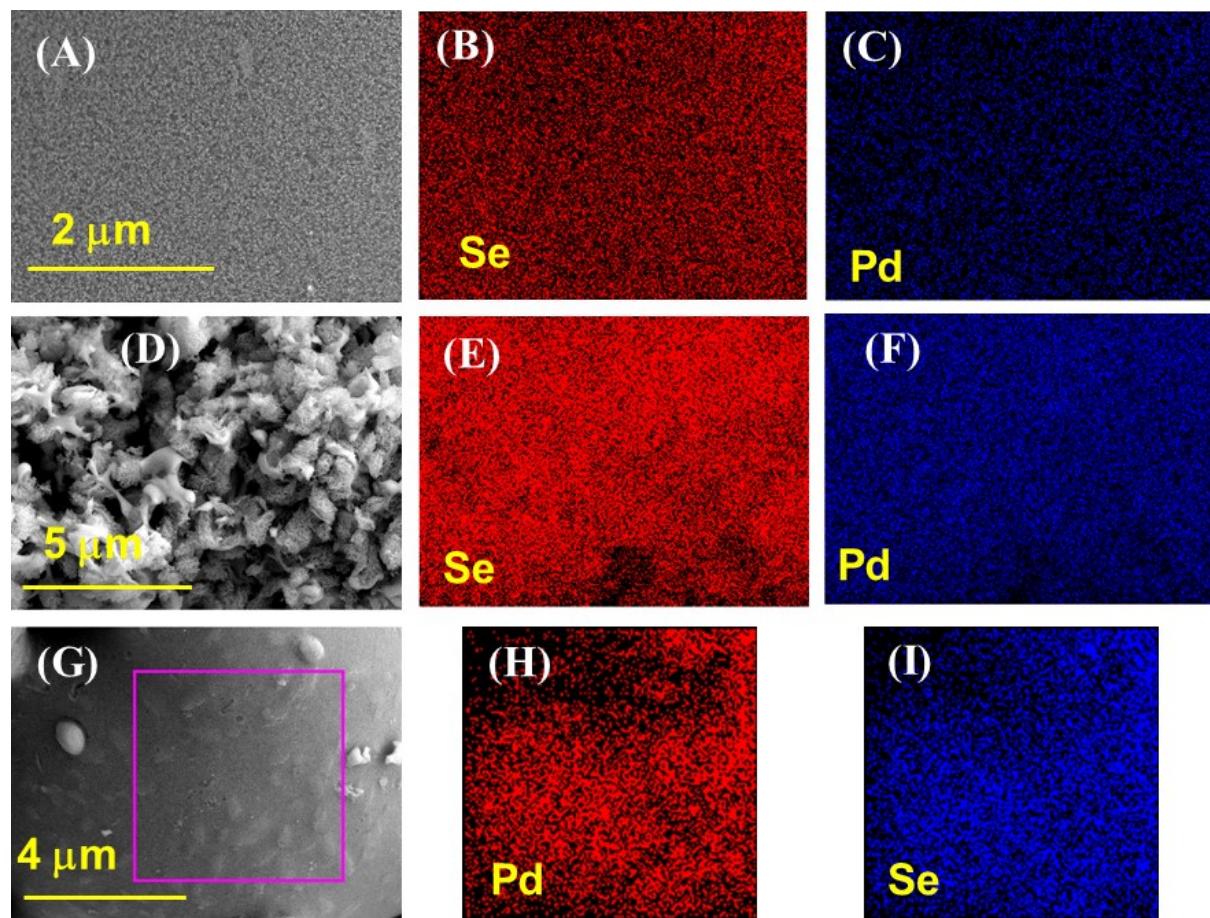


Fig. SI3 SEM images of (a) PSNP1, (b) PSNP2, (c) PSNP3; Elemental mapping of Selenium for (d) PSNP1, (e) PSNP2, (f) PSNP3 and palladium for (g) PSNP1, (h) PSNP2, (i) PSNP3

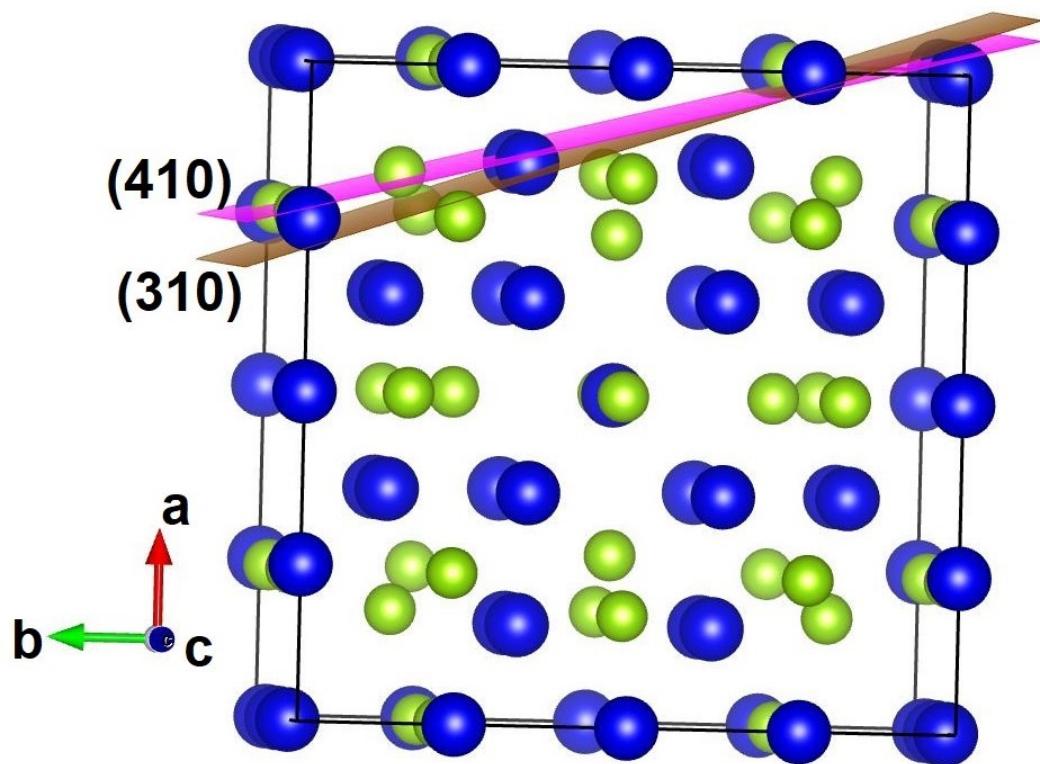


Fig. SI4. Unit cell of $\text{Pd}_{17}\text{Se}_{15}$ showing (310) and (413) planes

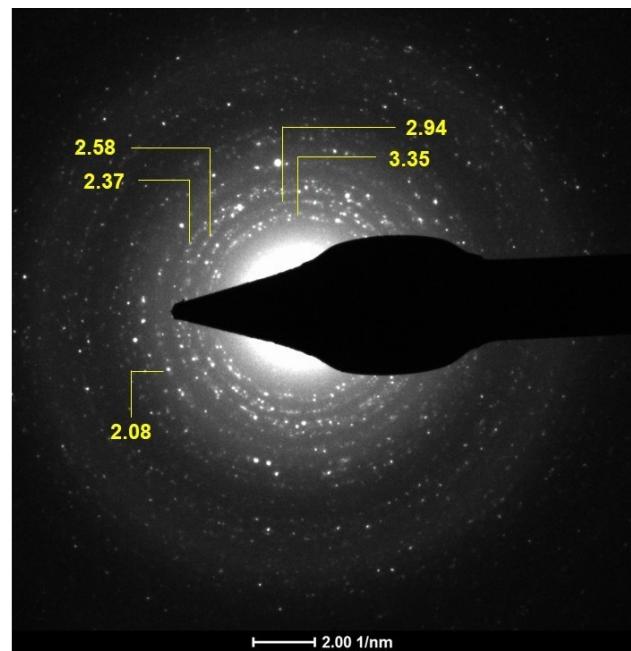


Fig. SI5A. SAED pattern of $\text{Pd}_{17}\text{Se}_{15}$ obtained from PdL1

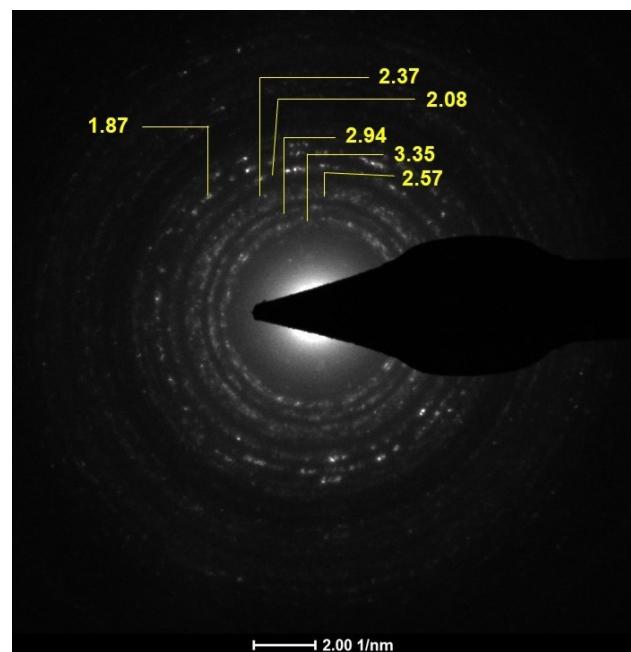


Fig. SI5B. SAED pattern of $\text{Pd}_{17}\text{Se}_{15}$ obtained from PdL2

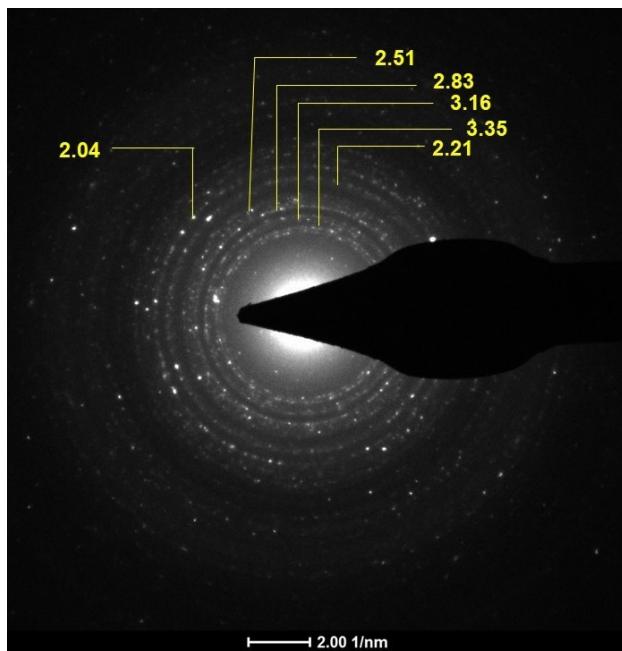


Fig. SI5C. SAED pattern of $\text{Pd}_{17}\text{Se}_{15}$ obtained from PdL3

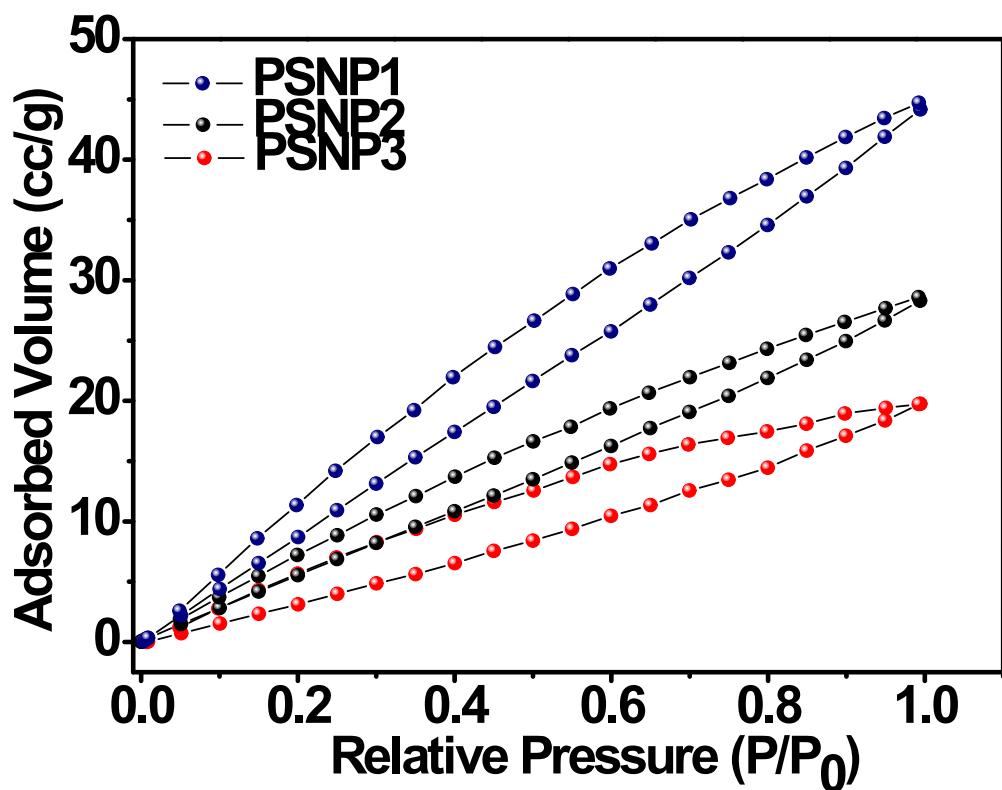


Fig. SI6A The N₂ adsorption-desorption isotherms

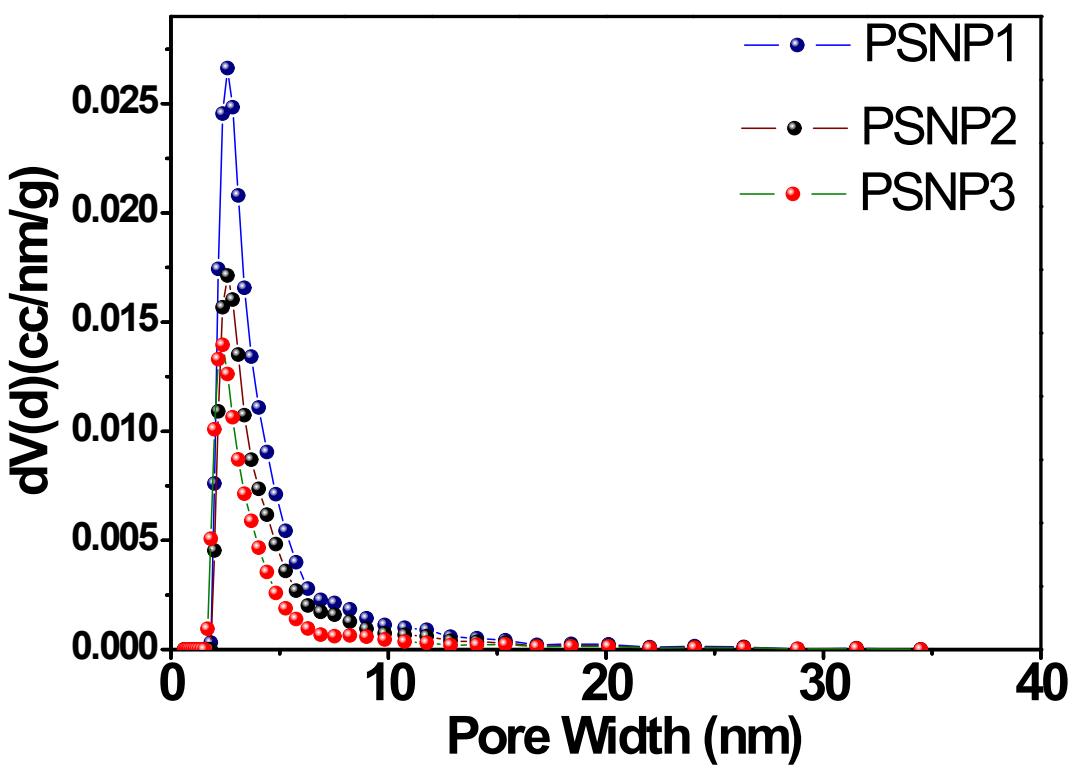


Fig. SI6B The pore size distributions (PSDs)

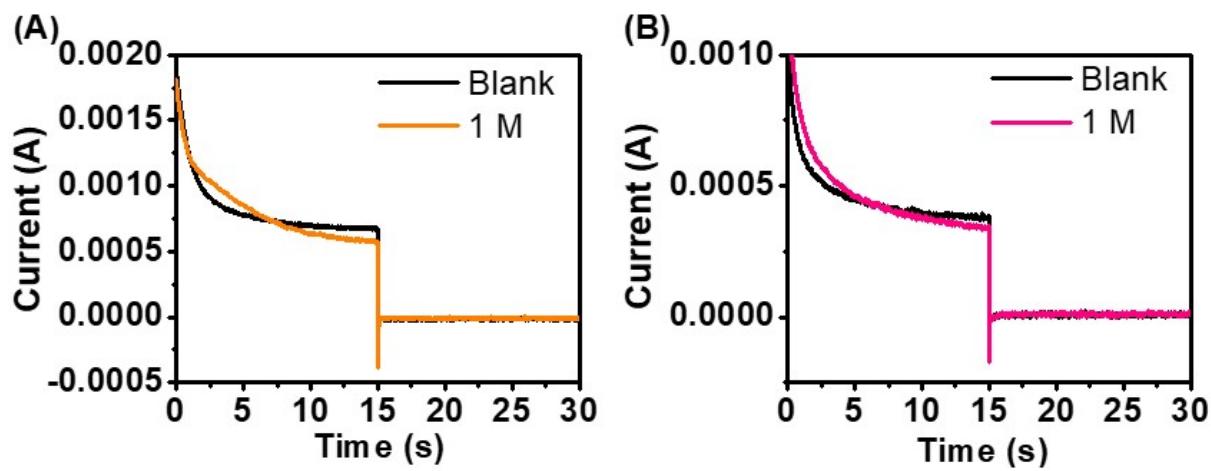


Fig. SI7 Chronoamperograms obtained at (A) PSNP2 modified electrode (B) PSNP3 modified electrode for 0 M and 1 M CH_3OH in 0.5 M NaOH. First and second applied potential were 800 mV and 0 mV vs. Ag/AgCl (3 M KCl).