Supplementary Information

Selectively activated suppressed quantum networks in self-assembled single atom-Ag catalyst-based room temperature sensors for health monitoring

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Contents

1. Synthesis of CdO as precursor and analyses of intermediate stages of CdS QD formation

CdO was synthesized by a standard precipitation technique.[1] In this method, a 1.0M solution of $Cd(NO_3)_2.4H_2O$ was prepared in DI water and ammonia solution was added dropwise till a yellowish precipitate was formed at pH 9. The mixture was centrifuged in wash ethanol medium to remove unreacted components and then dried at 60°C for 6 hours. The sample was then calcined at 400°C for 5 hours and ground finely to obtain a brownish powder. The sample was checked for formation of phase pure CdO by powder XRD.[1]

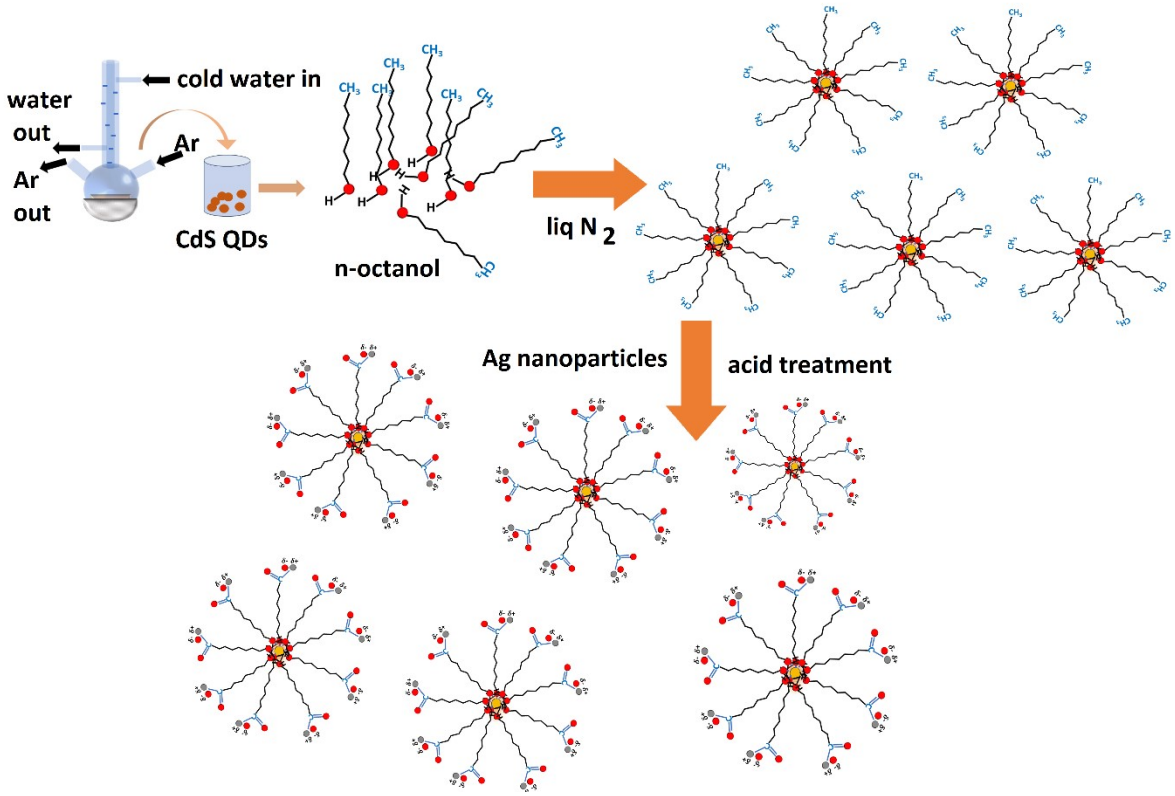

Figure S1: Schematic of the n-octanol assembly on CdS QDs and subsequent conversion to Ag@n-octanol(ox)@CdS QD assembly.

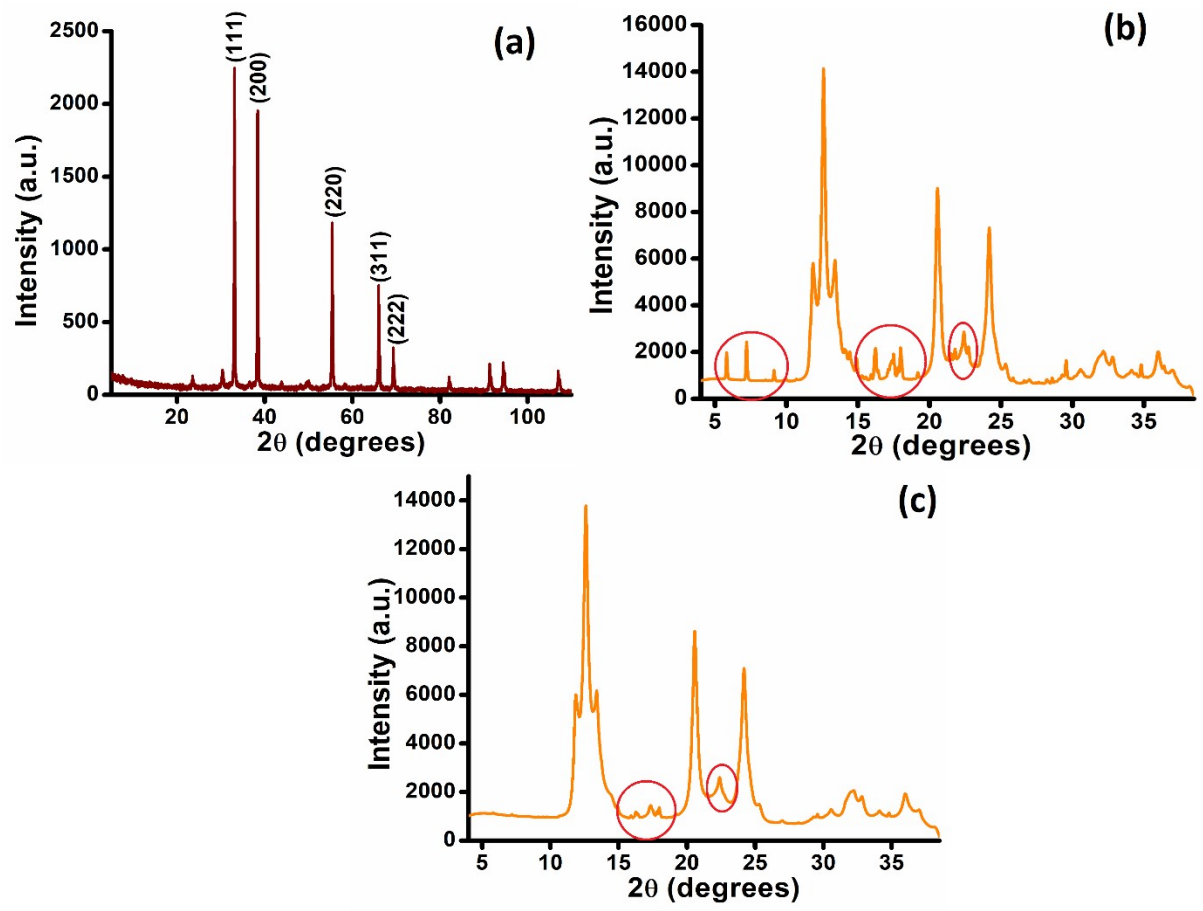

Figure S2: (a) Room temperature powder XRD of synthesized CdO for CdS QD preparation. (b-c) XRD patterns at intermediate stages of CdS QD formation with additional peaks highlighted in red circles.

Table S1: Ag precursor concentration vs. amount settled on the n-octanol(ox) substrate.

Sl. No.	Composition name	Ag solution (ml)	Ag:CdS (TEM EDX)
1	Ag@n-octanol(ox)@CdS QD_1	20	7%
2	Ag@n-octanol(ox)@CdS QD_2	40	4%
3	Ag@n-octanol(ox)@CdS QD_3	60	3.9%
4	Ag@n-octanol(ox)@CdS QD_4	80	4.1%

2. Electron microscopic studies

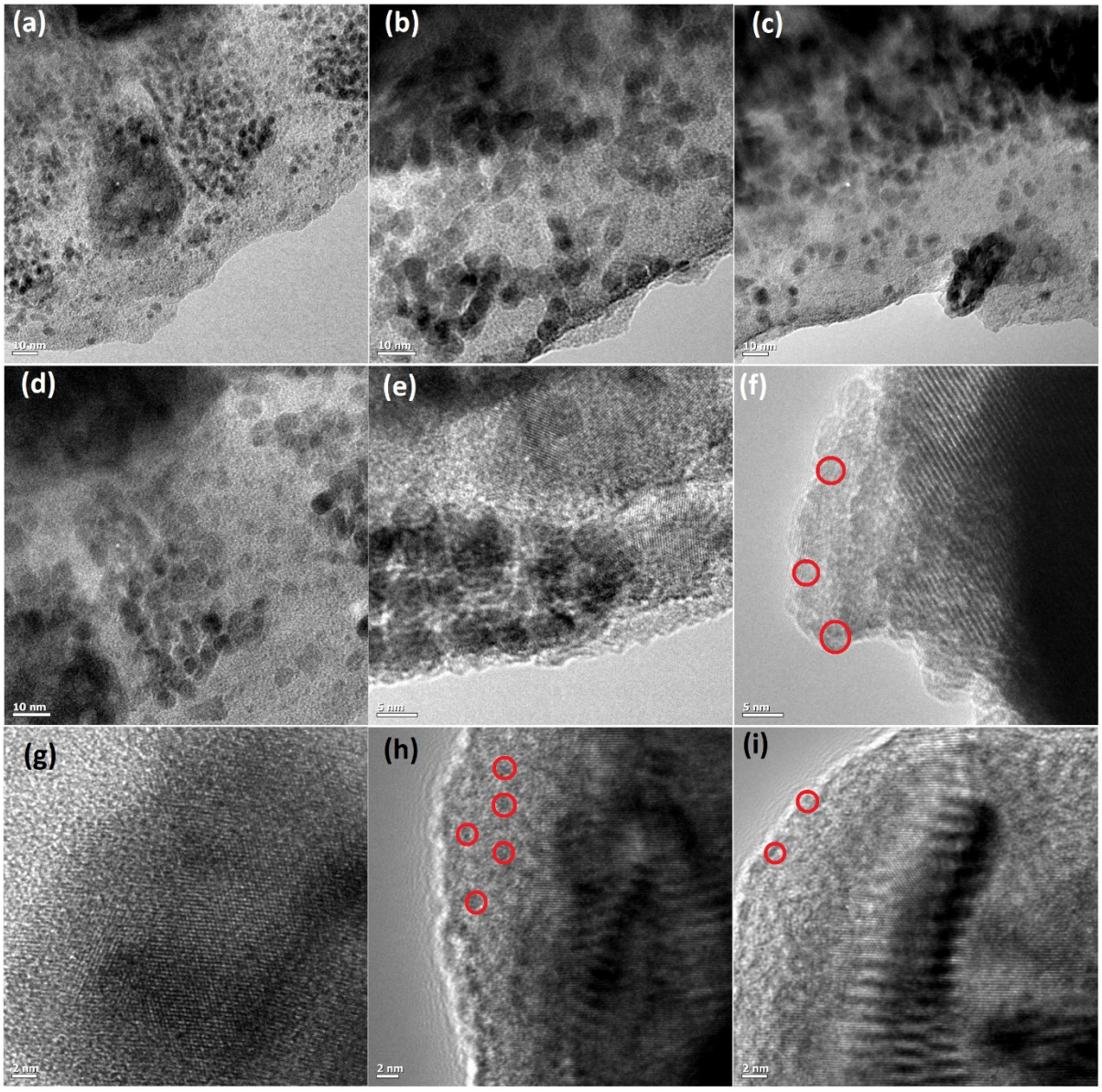

Figure S3: (a-c) Bright field TEM image of n-octanol@CdS QD assembly (d-e) Ag@n-octanol(ox)@CdS QD assembly (f-i) HRTEM images of Ag@n-octanol(ox)@CdS QD assembly with Ag highlighted in red circles.

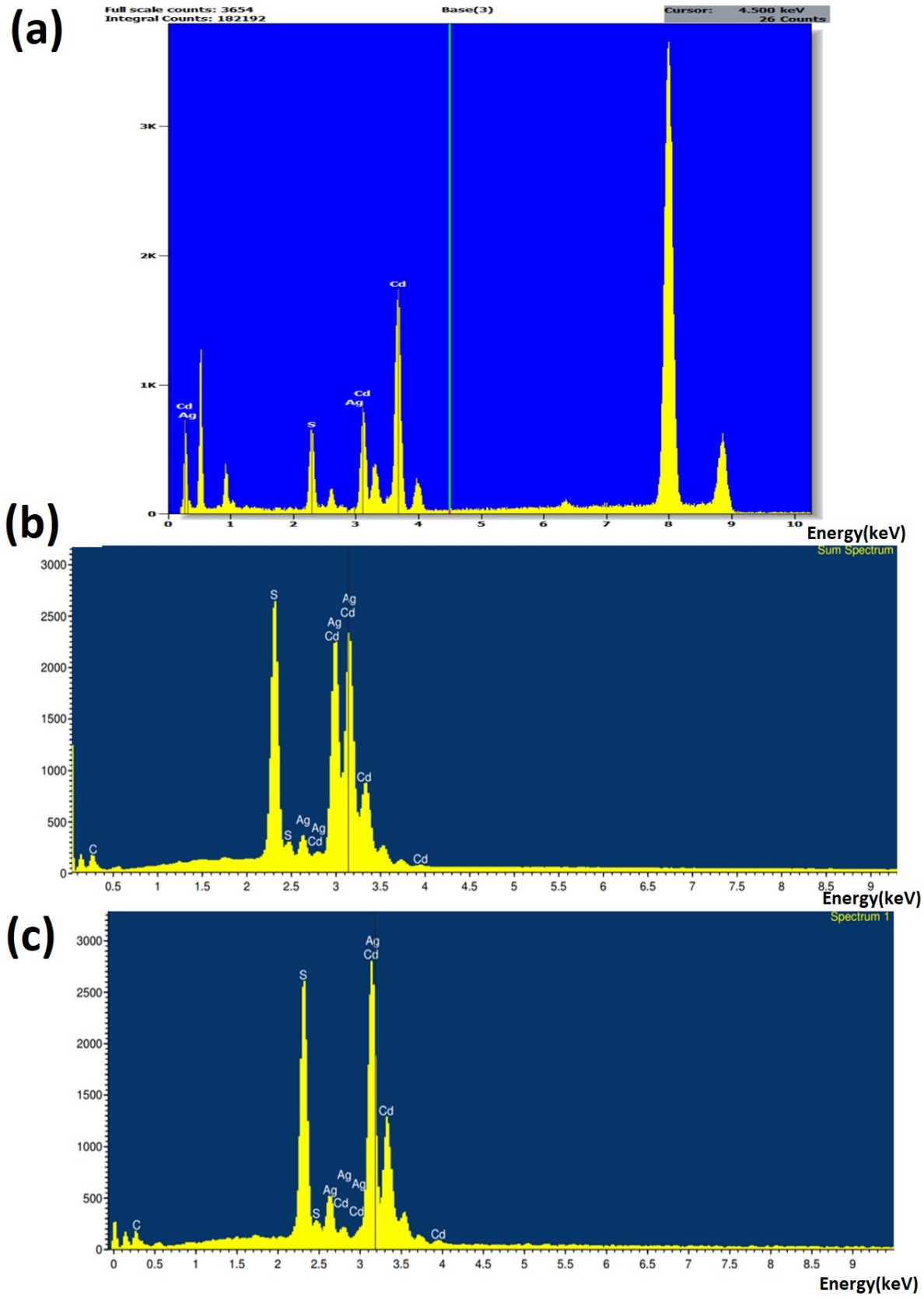

Figure S4: (a) TEM EDX spectrum of Ag@n-octanol(ox)@CdS QD_1 assembly with 7% Ag@CdS (w/w) (b-c) SEM EDX spectra of Ag@n-octanol(ox)@CdS QD_1 and Ag@n-

octanol(ox)@CdS QD_2 assembly with 7% Ag@CdS and 4% Ag@CdS (w/w) respectively. The spectra are taken from an average of 3 spots on the sample mounted.

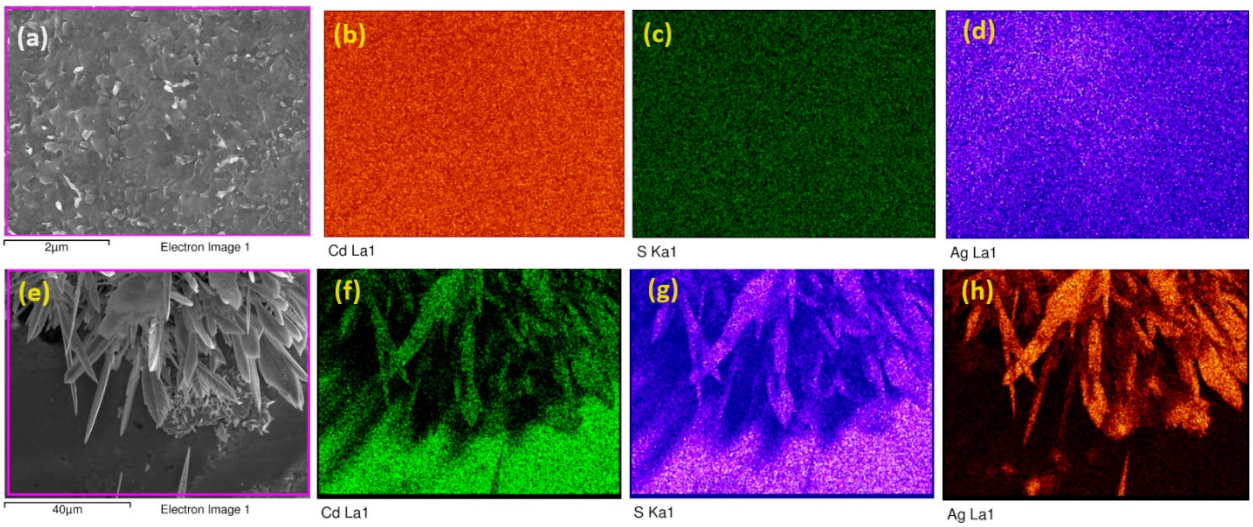

Figure S5: SEM color mapping of two different regions of the Ag@n-octanol(ox)@CdS QD_1 sample [(b-d) for region (a) and (f-h) for region (e)].

3. XPS analyses

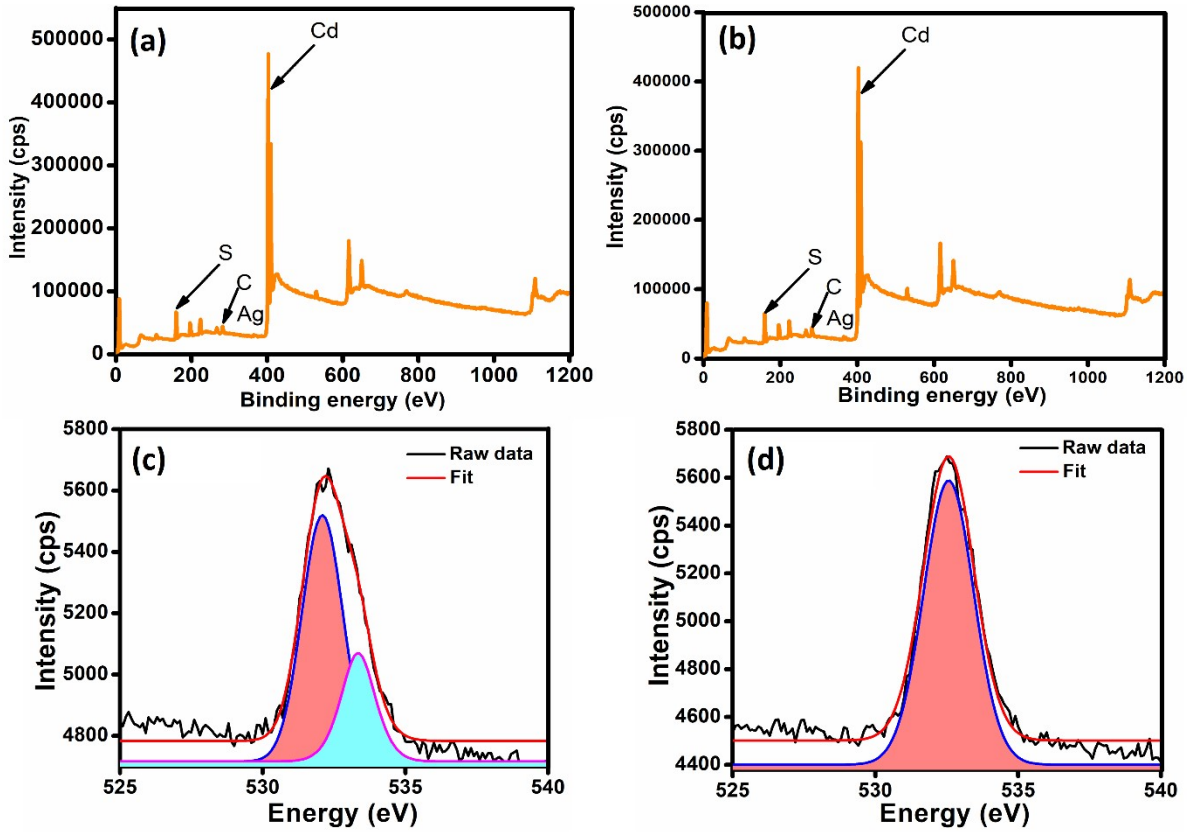

Figure S6: (a-b) Survey scan of Ag@n-octanol(ox)@CdS QD_1 and Ag@n-octanol(ox)@CdS QD_2 assembly with specific elements marked. (c-d) O1s core level spectra of Ag@n-octanol(ox)@CdS QD_2 and Ag@n-octanol(ox)@CdS QD_1 assembly. In (c) pink peak refers to O of -C=O and blue the surface hydroxyl groups. In (d) the O of -C=O

is prominent, but the hydroxyl signal gets hidden probably due to greater conversion of $-O^{-}H^{+}$ to $-O^{-}Ag^{+}$.[2]

4. XANES results

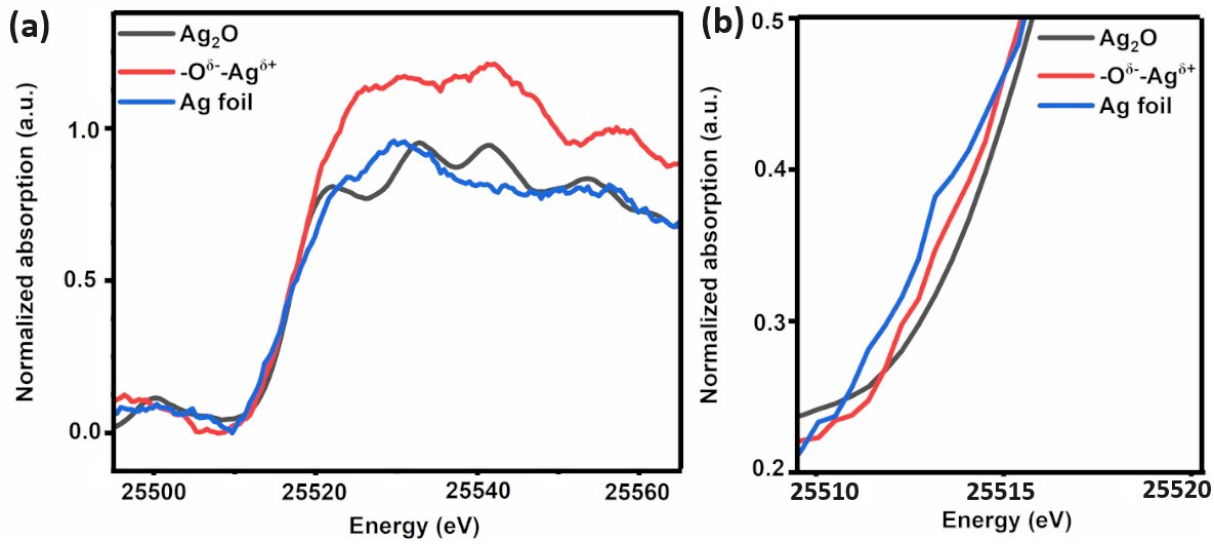

Figure S7: Ag K-edge XANES of (a) Ag foil, Ag_2O, Ag@n-octanol(ox)@CdS QD_1 (b) Enlarged region from 25.510 keV to 25.515 keV showing the edge for Ag@n-octanol(ox)@CdS QD_1 lying between Ag foil and Ag_2O.

5. Hall configuration

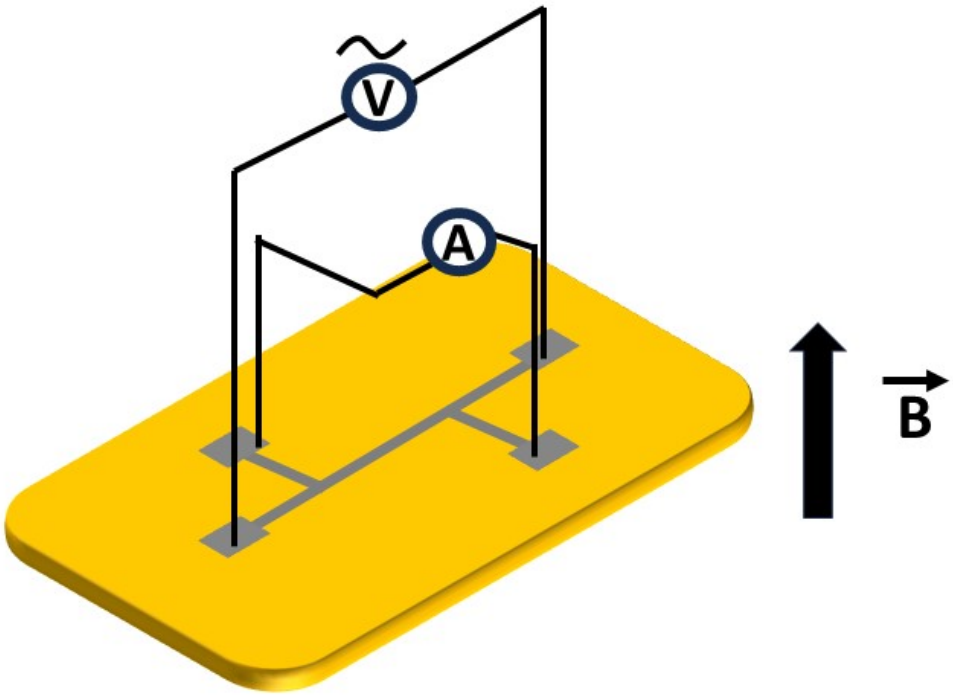

Figure S8: 4-probe Hall configuration of the sample.[3] V represents the voltage source and A the current meter. B is the applied magnetic field in a direction perpendicular to the sample plane. The grey lines are for representation purposes. The square contacts are made of silver. The length of the common is l = 2.3 mm and thickness of the pellet is d = 5mm. 4-probe resistivity has been calculated by standard formula of $R=\rho\frac{l}{A}$ where R is the resistance, ρ is the resistivity, l is the length of common region and A is the cross-sectional area A=l×d.

6. Sensing results

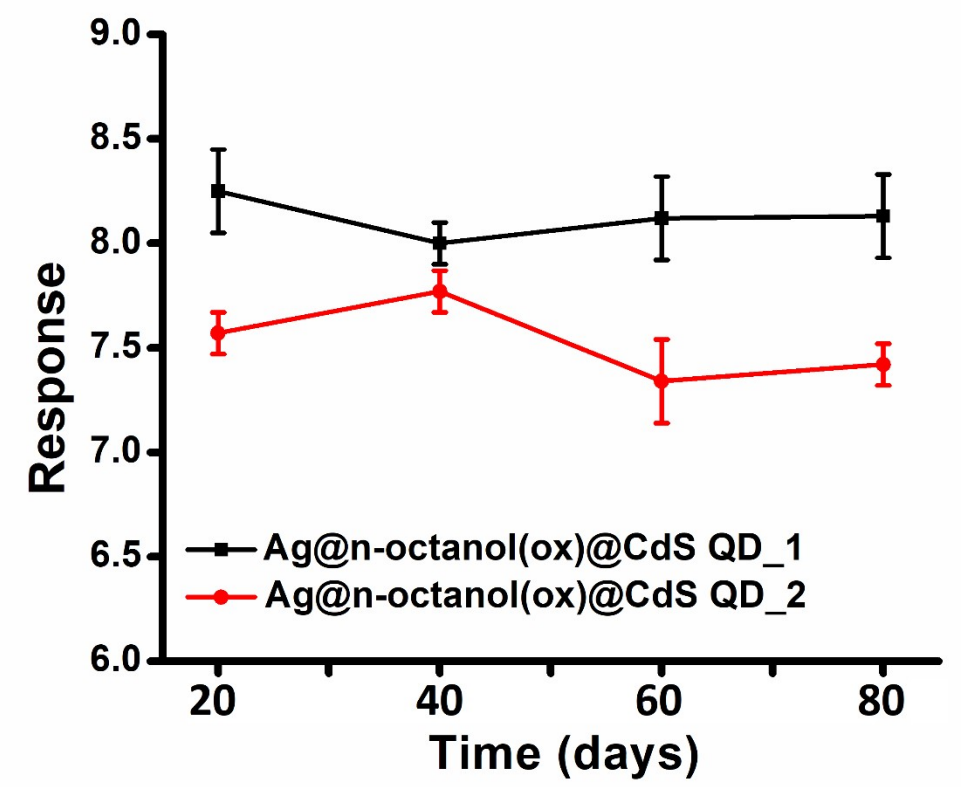

Figure S9: Repeatability of sensor samples with time for 500 ppb ethanol at room temperature.

7. PL measurements

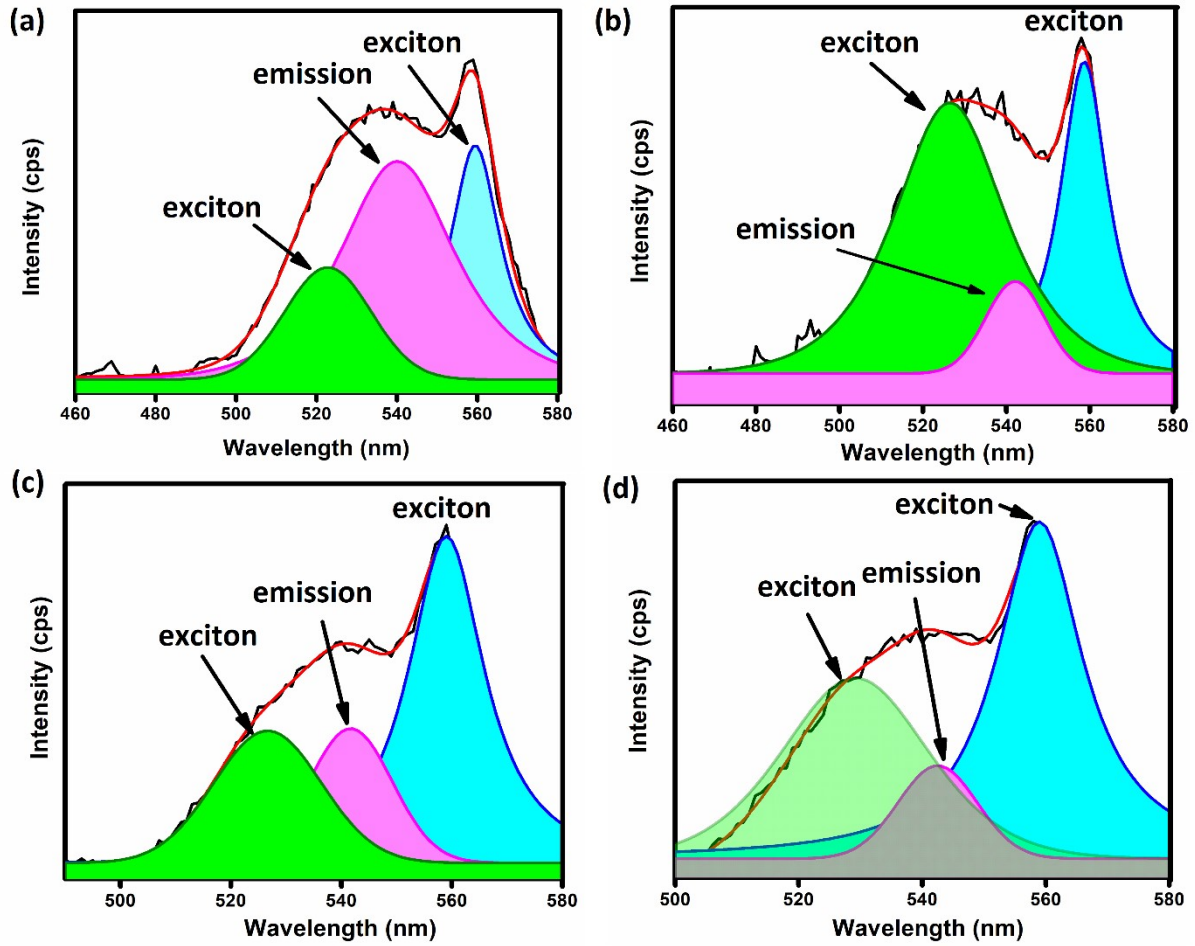

Figure S10: Low temperature PL spectra (78K) of (a) CdS QD (b) n-octanol@CdS QD, (c) Ag@n-octanol(ox)@CdS_1 and (d) Ag@n-octanol(ox)@CdS_2 samples respectively.

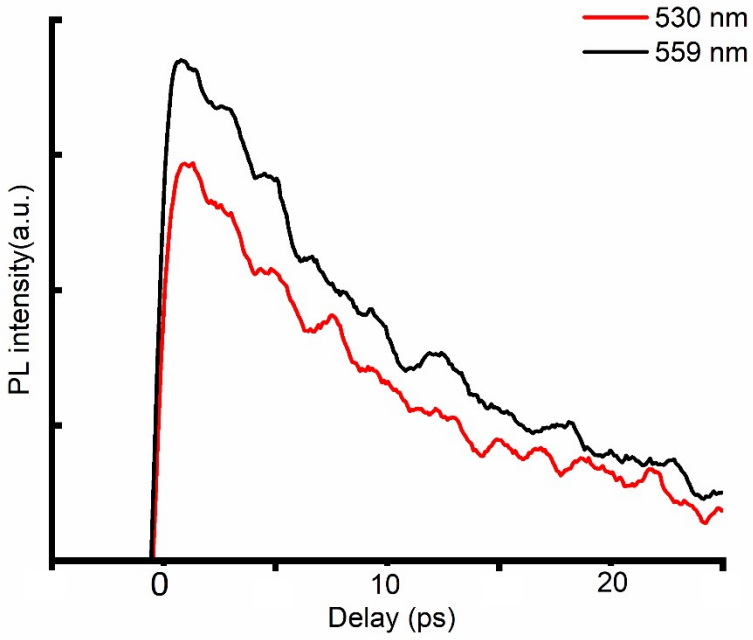

Figure S11: Lifetime measurement (78 K) of 530 nm emission and 559 nm emission in Ag@n-octanol(ox)@CdS_1 sample.

8. UV Vis spectroscopy

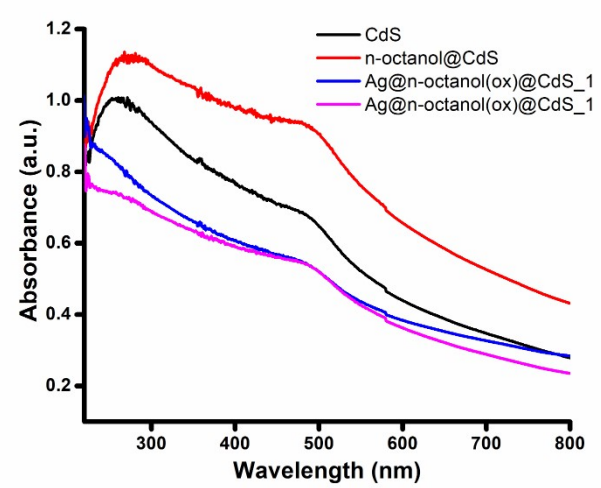

Figure S12: Room temperature UV Vis spectra of all samples in iso-propanol medium.

9. Ohmic characteristic analysis

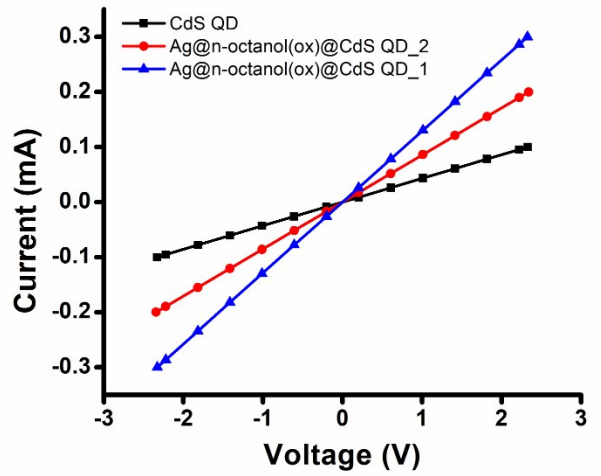

Figure S13: Room temperature I-V characteristics of sensor samples showing the ohmic nature of the sensors.

10. Control experiment schematic

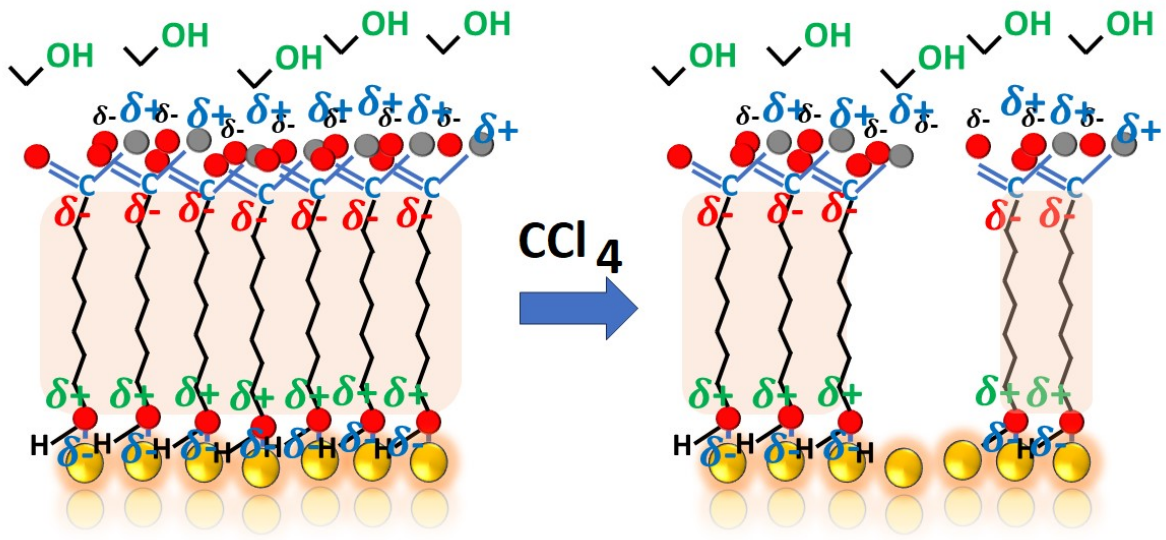

Figure S14: A small dent made on the encapsulation using CCl_4.[4] The capacitance measured was 1.5 µF with dissipation of 50%.

11. Impedance spectra

(i)

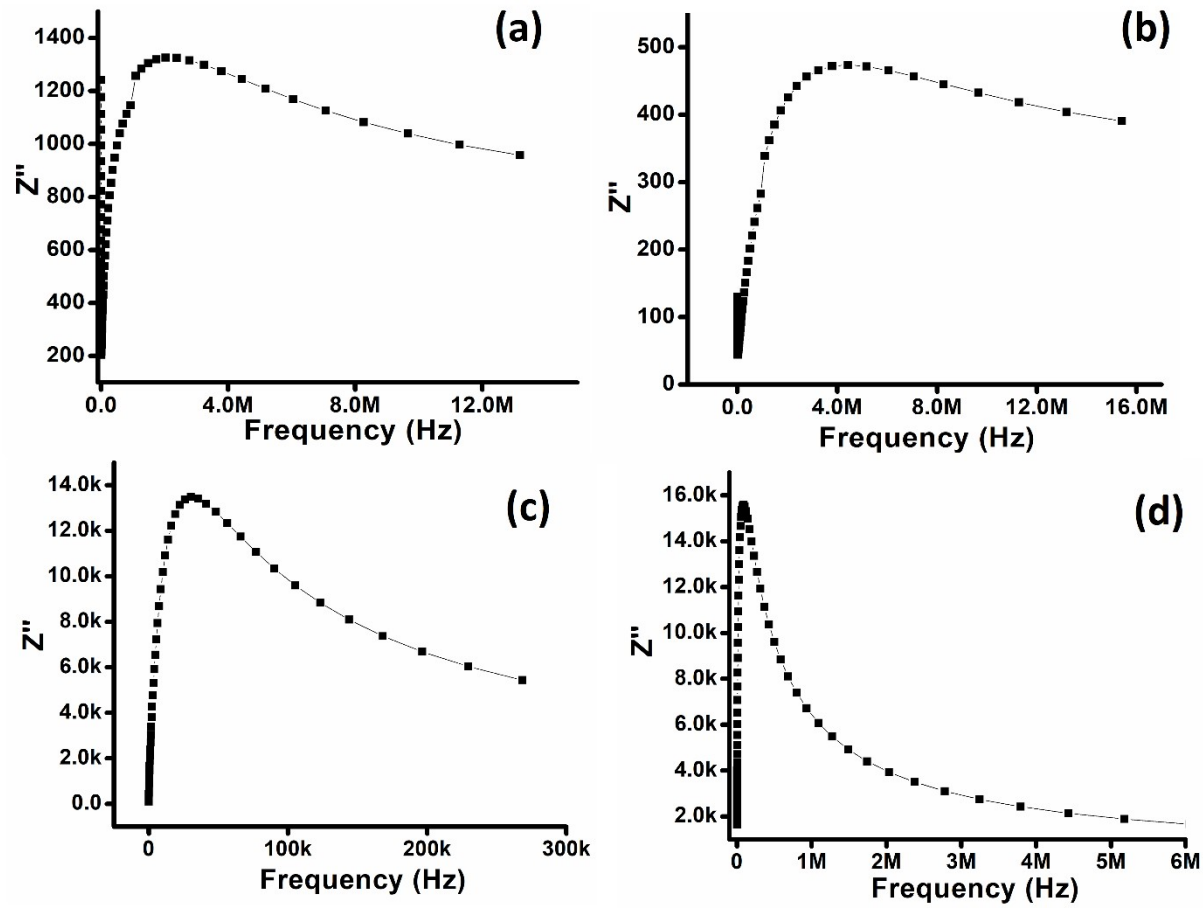

Figure S15: Capacitive reactance of (a, c) Ag@n-octanol(ox)@CdS_1 and (b, d) Ag@n-octanol(ox)@CdS_2 samples respectively in absence and presence of 200 ppm ethanol after 45 minutes of interaction

(ii)

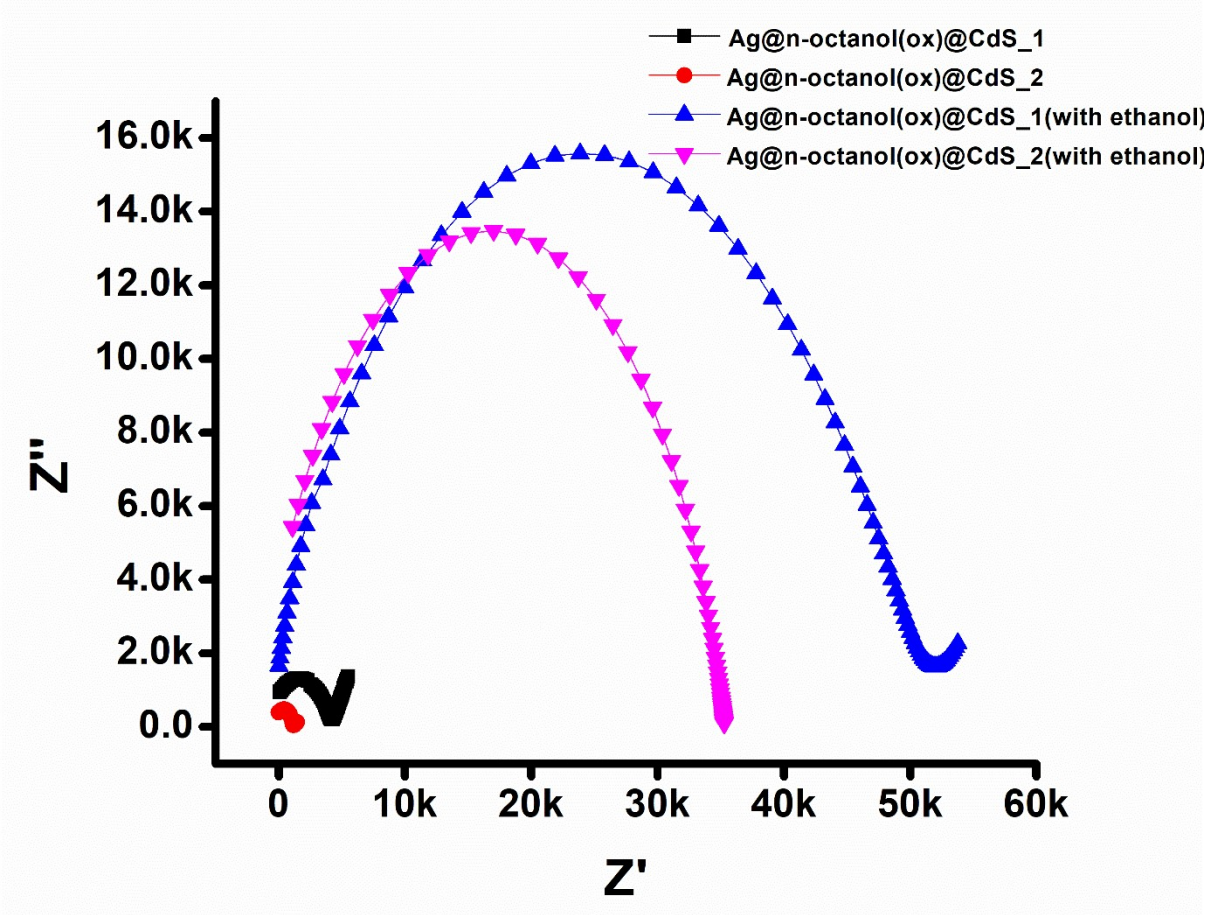

Figure S16: Nyquist plots[5] for the SACs in presence and absence of ethanol.

References

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