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

CdO was synthesized by a standard precipitation technique. In this method, a 1.0M solution of Cd(NO$_3$)$_2$.4H$_2$O 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.

**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.

<table>
<thead>
<tr>
<th>Sl. No.</th>
<th>Composition name</th>
<th>Ag solution (ml)</th>
<th>Ag: CdS (TEM EDX)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Ag@n-octanol(ox)@CdS QD_1</td>
<td>20</td>
<td>7%</td>
</tr>
<tr>
<td>2</td>
<td>Ag@n-octanol(ox)@CdS QD_2</td>
<td>40</td>
<td>4%</td>
</tr>
<tr>
<td>3</td>
<td>Ag@n-octanol(ox)@CdS QD_3</td>
<td>60</td>
<td>3.9%</td>
</tr>
<tr>
<td>4</td>
<td>Ag@n-octanol(ox)@CdS QD_4</td>
<td>80</td>
<td>4.1%</td>
</tr>
</tbody>
</table>
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 \(-\text{O}^+\text{H}^+\) to \(-\text{O}^\text{Ag}^+\).^{2}

4. XANES results

Figure S7: Ag K-edge XANES of (a) Ag foil, Ag\(_2\)O, 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\(_2\)O.
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 \(d = 5\) mm. 4-probe resistivity has been calculated by standard formula of \(R = \rho \frac{l}{A}\) where \(R\) is the resistance, \(\rho\) is the resistivity, \(l\) is the length of common region and \(A\) is the cross-sectional area \(A = l \times d\).
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

![UV Vis Spectra](image1)

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

9. Ohmic characteristic analysis

![I-V Characteristics](image2)

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$_4$. 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 for the SACs in presence and absence of ethanol.

**References**


