Supporting Information

Zn²⁺ induced Folding of RNA to produce Honeycomb like RNA -Mediated Fluorescing Zn²⁺/PbSe Nanostructures

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Figure S1a. Depth profile along X-axis in fresh SP1.



Figure S1b. Depth profile along Y-axis in fresh SP1.



Figure S1d. Depth profile along Y-axis in aged SP1.



Figure S2a. 2D and 3D AFM images of RNA mediated PbSe containing $[Zn^{2+}] = 1 \times 10^{-5}$ mol dm⁻³; Inset: Roughness histogram.



Figure S2b. 2D and 3D AFM images of PbSe containing $[Zn^{2+}] = 2.5 \times 10^{-5}$ mol dm⁻³;Inset: Roughness histogram.



Figure S2c. 2D and 3D AFM images of RNA mediated PbSe containing $[Zn^{2+}] = 5 \times 10^{-5} \text{ mol dm}^{-3}$; Inset: Roughness histogram.



Figure S2d. 2D and 3D AFM images of RNA mediated PbSe containing $[Zn^{2+}] = 15.0 \times 10^{-5} \text{ mol dm}^{-3}$; Inset: Roughness histogram.



Figure S3A. 2D AFM images of SB1: Fresh (a); Aged (a')



Figure S3B. 3D AFM images of SB1: Fresh (a); Aged (a') Inset: Roughness histogram.



Figure S3C. Histogram showing pores/ grains analysis of SB1: Fresh (a); Aged (a´).



| Element | Wt% | At% |
|---------|------------|-------|
| СК | 63.33 | 84.54 |
| NK | 11.09 | 12.69 |
| SeL | 03.47 | 00.70 |
| ZnK | 02.11 | 00.52 |
| PbL | 20.00 | 01.55 |
| Matrix | Correction | ZAF |



Figure S4a. EDAX analysis of FESEM images of fresh SP1.



| Element | Wt% | At% |
|---------|------------|-------|
| СК | 69.28 | 85.67 |
| NK | 11.57 | 12.27 |
| SeL | 03.29 | 00.62 |
| ZnK | 01.95 | 00.44 |
| PbL | 13.91 | 01.00 |
| Matrix | Correction | ZAF |



Figure S4b. EDAX analysis of FESEM images of fresh SP1.



| Element | Wt% | At% |
|---------|------------|-------|
| СК | 50.51 | 67.13 |
| NK | 24.61 | 28.05 |
| ZnL | 08.04 | 01.96 |
| SeL | 05.39 | 01.09 |
| РК | 02.03 | 01.05 |
| PbM | 09.42 | 00.73 |
| Matrix | Correction | ZAF |



Figure S4c. EDAX analysis of FESEM images of aged SP1.



| Element | Wt% | At% |
|---------|------------|-------|
| СК | 57.77 | 74.33 |
| NK | 18.83 | 20.77 |
| ZnL | 13.76 | 03.25 |
| SeL | 01.66 | 00.33 |
| РК | 01.71 | 00.85 |
| PbM | 06.26 | 00.47 |
| Matrix | Correction | ZAF |



Figure S4d. EDAX analysis of FESEM images of aged SP1.



Figure S5a. 3D view of TEM image of Fresh SP1 recorded with the help of *image J* software.



Figure S5a'. 3D view of TEM image of aged SP1 recorded with the help of *imageJ* software.



Building Block of SP1

Assembly of Building Block (SP1)

Scheme S1. Interactions of RNA in the absence (SB1) and presence of PbSe (SP1) forming Building Block and their Assembly.

| Sample | Peaks /orbital | B.E. (eV) Literature in reference to PbSe | B.E. (eV) Observed |
|--|--|--|------------------------------|
| Zn ²⁺ /PbSe | Pb 4f _{7/2} Pb 4f _{5/2} | 142.5 137.3 | 141.2 136.4 |
| Zn ²⁺ /PbSe | Se 3d _{5/2} Se 3d _{3/2} | 53.3 54.18 | 51.2 54.1 |
| Pb(OH) ₂ in Zn ²⁺ /PbSe | Ols | 530.8 | 529.1 |
| Zn(OH) ₂ | O1s | 532.3 | 534.0 |

Table S1. XPS spectral data

Table S2. Depth and hole/pore analysis of SP1 in AFM images shown in Figure 4.

| Sample | No. of pores | Size of pore | Depth along | Depth along | Surface |
|------------|--------------|--------------|-------------|-------------|-----------|
| | | (nm) | X-axis (nm) | Y-axis(nm) | roughness |
| | | | | | (nm) |
| SP1(Fresh) | 139 | 4.3 | 1-3 | 3.0 | 5.2 |
| SP1(Aged) | 305 | 5.3 | 1.5-3 | 4.0 | 5.4 |

Table S3. Depth and pore/ grain analysis of SB1 in AFM images shown in Figure S3a.

| Sample | No. of pores / grains | Size of pores / grains (nm) |
|------------|-----------------------|-----------------------------|
| SB1(Fresh) | 96 pores | 11.1 |
| SB1(Aged) | 1022 grains | 3.3 |

| Moiety/Functional | Vibrational bands in cm ⁻¹ | | |
|-------------------------------|---------------------------------------|--------------|-------------|
| group | SB | SB1 | SP1 |
| In plane | 1693 (br) | disappeared | disappeared |
| vibrations: G&U | | | |
| A&C | 1642 (m) | 1644(br) | 1649 (s) |
| G | 1544 (m) | disappeared | disappeared |
| U (medium) | 1469 (m) | 1488(br) | 1492 (sh) |
| In plane C2´-OH | 1421(br) | 1414 (br,m) | 1411(s) |
| Purine in anti | 1385(s) | disappeared | disappeared |
| confm. | | | |
| Purine in syn | 1360 (sh) | 1340 (br) | 1340 (m) |
| confm. | | | |
| С | 1281 (sh) | 1281(br) | disappeared |
| Assym. Stretch | 1227 (s,br) | 1244 (m,br) | 1242(m,br) |
| PO ₂ ²⁻ | | | |
| CO stretch of | 1070(s) | 1084(br, sh) | 1089(m) |
| backbone | | | |
| Ribose vib. due to | 996 (br) | disappeared | disappeared |
| 2´-ОН | | | |
| RNA backbone | 966 (m) | 966 (br) | 970(sh) |

Table S4. Mid IR spectral data of SB, SB1, and SP1.

s-strong; m- medium; w- weak; sh- shoulder; br- broad.

| | Chemical Shift (δ) (ppm) | | | |
|---|--------------------------|--|----------------------------|--|
| Moieties | (SB)* | SB1 | SP1 | |
| | RNA | RNA-Zn ²⁺ +Pb ²⁺ | RNA-Zn ²⁺ /PbSe | |
| Sugar protons (H ₂ ', | 4.05 - 4.08 | 4.35 -3.41 | 4.49 -3.75 | |
| $H_{3}', H_{4}', H_{5}', H_{5}'')$ | | | | |
| bases and sugar | 6.11-6.33 | 5.70 - 5.98 | 5.83-6.07 | |
| protons $(\mathbf{H}_{1}', \mathbf{H}_{5})$ | | | | |
| aromatic protons of | | | | |
| purine and | 7.63 -8.66 | 7.63-8.33 | 7.65-8.46 | |
| pyrimidine bases (H ₂ , | | | | |
| H ₈ , H ₆) | | | | |
| Sugar 2'-OH | 2.41 | 1.80 | 1.93 | |
| ³¹ P | -0.89 | -0.84 | -0.82 | |

Table S5. ¹H NMR and ³¹P NMR spectral data of SB, SB1, and SP1:

*Ref. 14

Table S6. CD spectral data of SB, SB1, and SP1:

| Sample | Peak 1 | Peak 2 | Peak 3 |
|-----------|-------------|-------------|-------------|
| SB1 Fresh | X = 211.98, | X = 241.77, | X = 272.55, |
| | Y = -3.35 | Y = -1.68 | Y = 3.34 |
| SP1 Fresh | X = 209.28, | X = 242.10, | X = 271.86, |
| | Y = -3.50 | Y = -1.48 | Y = 3.59 |
| SP1 Aged | X = 207.99, | X = 240.42, | X = 271.53, |
| | Y = -0.73 | Y = -1.08 | Y = 2.81 |

X = Wavelength (nm), Y= Ellipticity