

Electronic Supplementary Information

***In situ* synthesis of [Cu(BODN)·5H₂O]_n@nano-Al composite energetic films with tunable properties in pyro-MEMS**

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1. Schematic diagram for preparing $[\text{Cu}(\text{BODN})\cdot 5\text{H}_2\text{O}]_n$ single crystal

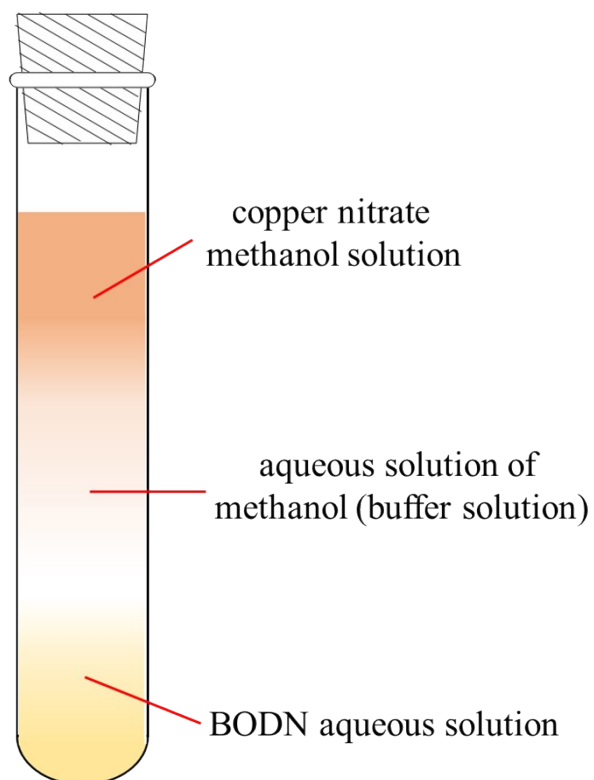


Fig. S1 Schematic diagram for preparing $[\text{Cu}(\text{BODN})\cdot 5\text{H}_2\text{O}]_n$ single crystal by liquid-phase diffusion method

2. Single-crystal X-ray Diffraction Analysis of [Cu(BODN)·5H₂O]_n

Table S1 Selected bond lengths [Å] of [Cu(BODN)·5H₂O]_n

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|-----------------|------------------|----------|----------------|----------------|----------|
| Cu ¹ | O ³ | 1.992(2) | N ⁶ | C ⁴ | 1.314(4) |
| Cu ¹ | O ⁴ | 1.971(2) | O ² | N ⁸ | 1.228(4) |
| Cu ¹ | O ¹¹¹ | 2.310(3) | N ⁵ | C ³ | 1.282(4) |
| Cu ¹ | N ⁶ | 1.986(3) | N ³ | N ⁴ | 1.403(4) |
| Cu ¹ | N ³¹ | 1.980(3) | N ³ | C ¹ | 1.315(4) |
| Cu ¹ | O ¹ | 2.261(3) | O ¹ | N ⁸ | 1.245(4) |
| O ⁹ | C ¹ | 1.367(4) | N ⁴ | C ² | 1.281(4) |
| O ⁹ | C ² | 1.353(4) | N ⁷ | N ⁸ | 1.342(3) |
| O ⁵ | C ⁴ | 1.371(4) | N ⁷ | C ⁴ | 1.340(4) |
| O ⁵ | C ³ | 1.357(4) | N ¹ | N ² | 1.338(4) |
| O ¹¹ | N ¹ | 1.251(4) | N ² | C ¹ | 1.343(4) |
| O ¹⁰ | N ¹ | 1.238(4) | C ³ | C ² | 1.446(4) |
| N ⁶ | N ⁵ | 1.401(4) | | | |

Table S2 Selected bond angles [°] of [Cu(BODN)·5H₂O]_n

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|-----------------|-----------------|------------------|------------|-----------------|----------------|-----------------|----------|
| O ³ | Cu ¹ | O ¹¹¹ | 90.19(10) | C ¹ | N ³ | N ⁴ | 107.7(2) |
| O ³ | Cu ¹ | O ¹ | 92.05(11) | N ⁸ | O ¹ | Cu ¹ | 135.8(2) |
| O ⁴ | Cu ¹ | O ³ | 178.63(11) | C ² | N ⁴ | N ³ | 104.6(3) |
| O ⁴ | Cu ¹ | O ¹¹¹ | 88.60(10) | C ⁴ | N ⁷ | N ⁸ | 116.1(3) |
| O ⁴ | Cu ¹ | N ⁶ | 89.25(10) | O ² | N ⁸ | O ¹ | 120.0(3) |
| O ⁴ | Cu ¹ | N ³¹ | 90.48(10) | O ² | N ⁸ | N ⁷ | 116.7(3) |
| O ⁴ | Cu ¹ | O ¹ | 89.18(11) | O ¹ | N ⁸ | N ⁷ | 123.2(3) |
| N ⁶ | Cu ¹ | O ³ | 90.44(10) | O ¹¹ | N ¹ | N ² | 123.5(3) |
| N ⁶ | Cu ¹ | O ¹¹¹ | 104.76(10) | O ¹⁰ | N ¹ | O ¹¹ | 120.5(3) |
| N ⁶ | Cu ¹ | O ¹ | 77.15(10) | O ¹⁰ | N ¹ | N ² | 116.0(3) |
| N ³¹ | Cu ¹ | O ³ | 89.87(10) | N ¹ | N ² | C ¹ | 116.6(3) |
| N ³¹ | Cu ¹ | O ¹¹¹ | 76.96(10) | N ⁶ | C ⁴ | O ⁵ | 110.2(3) |
| N ³¹ | Cu ¹ | N ⁶ | 178.26(12) | N ⁶ | C ⁴ | N ⁷ | 137.3(3) |
| N ³¹ | Cu ¹ | O ¹ | 101.12(10) | N ⁷ | C ⁴ | O ⁵ | 112.5(3) |
| O ¹ | Cu ¹ | O ¹¹¹ | 177.05(9) | N ³ | C ¹ | O ⁹ | 110.2(3) |
| C ² | O ⁹ | C ¹ | 102.9(2) | N ³ | C ¹ | N ² | 137.5(3) |
| C ³ | O ⁵ | C ⁴ | 102.9(2) | N ² | C ¹ | O ⁹ | 112.3(3) |
| N ¹ | O ¹¹ | Cu ¹² | 134.4(2) | O ⁵ | C ³ | C ² | 119.3(3) |
| N ⁵ | N ⁶ | Cu ¹ | 121.4(2) | N ⁵ | C ³ | O ⁵ | 114.2(3) |
| C ⁴ | N ⁶ | Cu ¹ | 129.8(2) | N ⁵ | C ³ | C ² | 126.5(3) |
| C ⁴ | N ⁶ | N ⁵ | 107.8(2) | O ⁹ | C ² | C ³ | 117.1(3) |
| C ³ | N ⁵ | N ⁶ | 104.9(3) | N ⁴ | C ² | O ⁹ | 114.5(3) |
| N ⁴ | N ³ | Cu ¹² | 121.1(2) | N ⁴ | C ² | C ³ | 128.3(3) |
| C ¹ | N ³ | Cu ¹² | 130.3(2) | | | | |

3. Morphologies of the samples prepared under different conditions

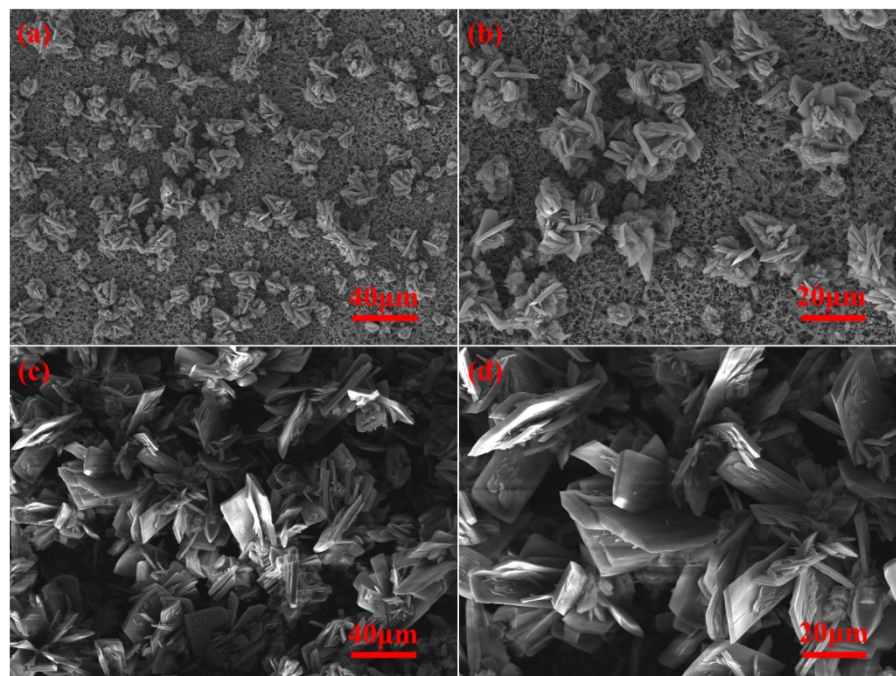


Fig. S2 (a) and (b) represent low and high magnification SEM images of $[\text{Cu}(\text{BODN})\cdot 5\text{H}_2\text{O}]_n$ arrays prepared by reaction for 5 min, (c) and (d) represent low and high magnification SEM images of $[\text{Cu}(\text{BODN})\cdot 5\text{H}_2\text{O}]_n$ arrays prepared by reaction for 20 min.

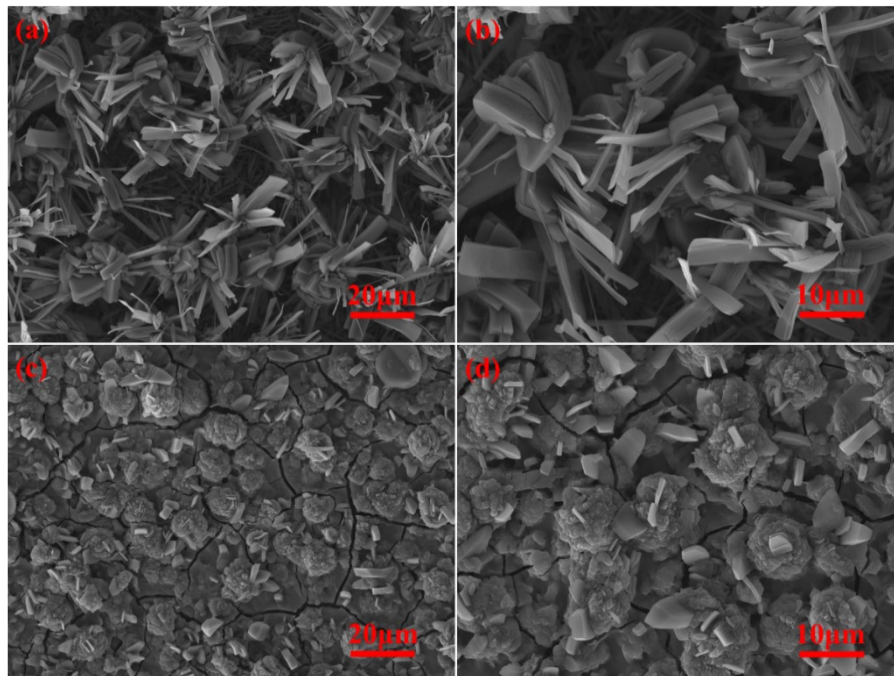


Fig. S3 (a) and (b) represent the low and high magnification SEM images of $[\text{Cu}(\text{BODN})\cdot 5\text{H}_2\text{O}]_n$ arrays prepared at a solution concentration of $2 \text{ g}\cdot\text{L}^{-1}$, (c) and (d) represent the low and high magnification SEM images of $[\text{Cu}(\text{BODN})\cdot 5\text{H}_2\text{O}]_n$ arrays prepared at a solution concentration of $6 \text{ g}\cdot\text{L}^{-1}$.

4. The TG curve of $[\text{Cu}(\text{BODN})\cdot 5\text{H}_2\text{O}]_n$ crystals

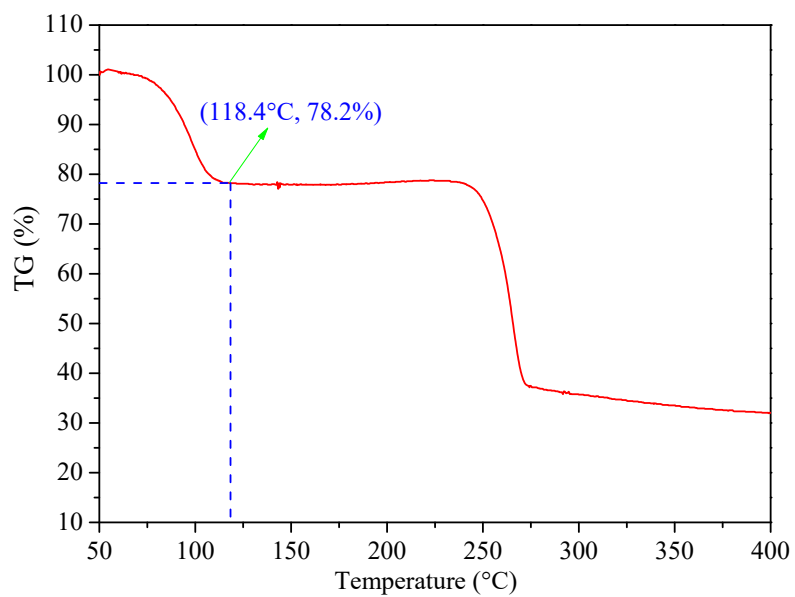


Fig. S4 The TG curve of $[\text{Cu}(\text{BODN})\cdot 5\text{H}_2\text{O}]_n$ crystals

5. The composition of energetic films estimated by the heat releases

Table S3 The composition of energetic films estimated by the heat releases

| Samples | Cu(OH) ₂ (%) | [Cu(BODN)·5H ₂ O] _n (%) | Al (%) | Nitrocellulose (%) |
|--|----------------------------|--|-----------|-----------------------|
| [Cu(BODN)·5H ₂ O] _n arrays (5 min) | 34.6 | 65.4 | -- | -- |
| [Cu(BODN)·5H ₂ O] _n arrays (10 min) | 0 | 100 | -- | -- |
| [Cu(BODN)·5H ₂ O] _n @nano-Al (2 drops) | -- | 86.2 | 11.7 | 2.1 |
| [Cu(BODN)·5H ₂ O] _n @nano-Al (6 drops) | -- | 72.1 | 23.7 | 4.2 |