

# Facilitated Explosion of Nitro Compound Confined in Metal-Organic Frameworks

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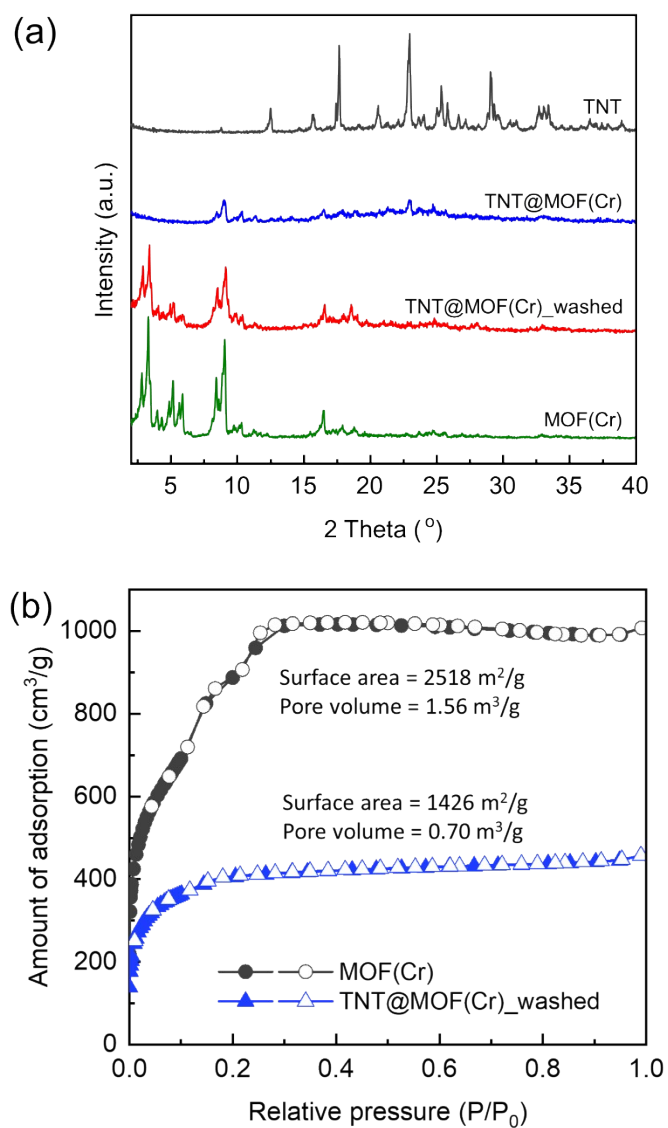
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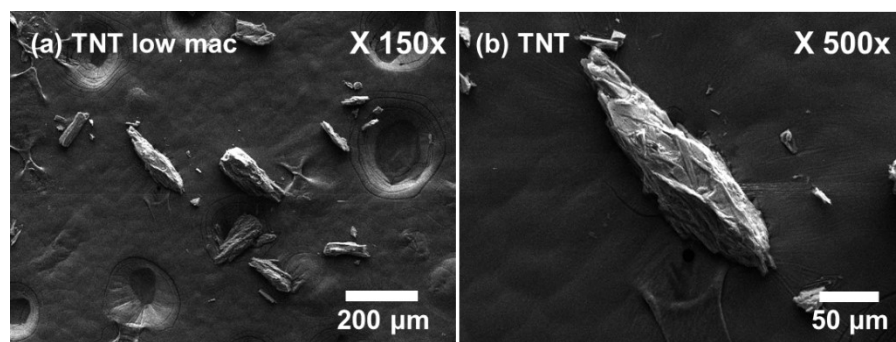
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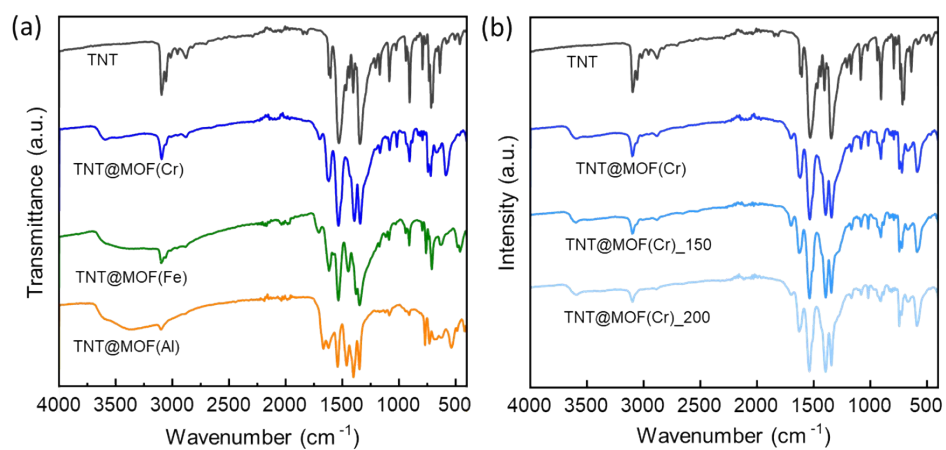
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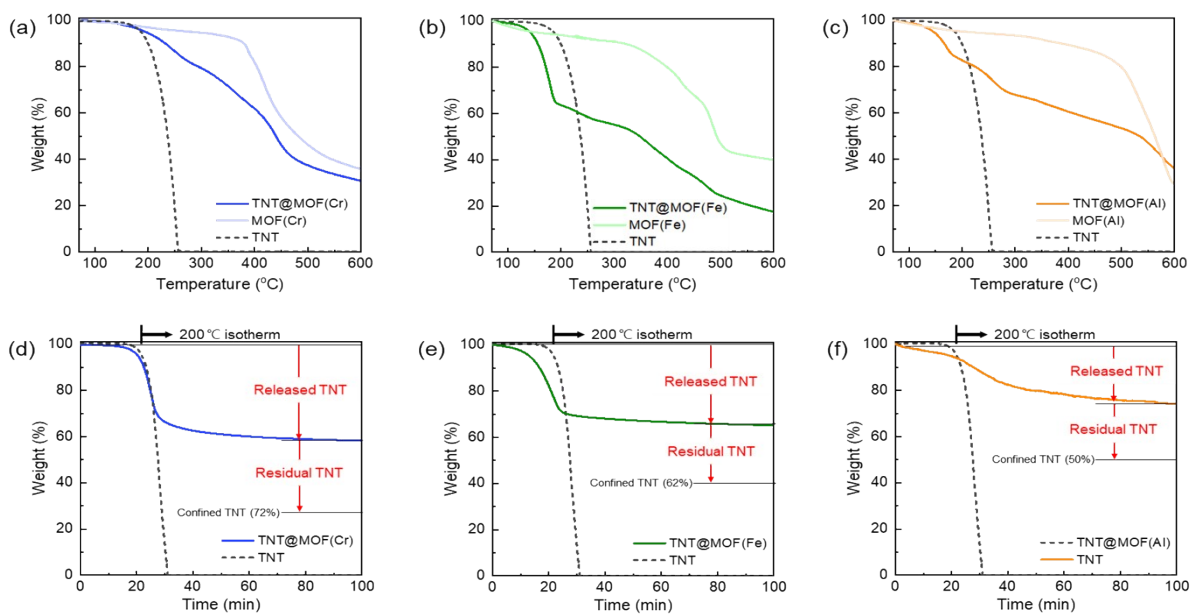
**Figure S1.** (a) XRD peaks and (b)  $\text{N}_2$  isotherm of TNT, TNT@MOF(Cr), TNT@MOF(Cr)\_washed, and MOF(Cr).



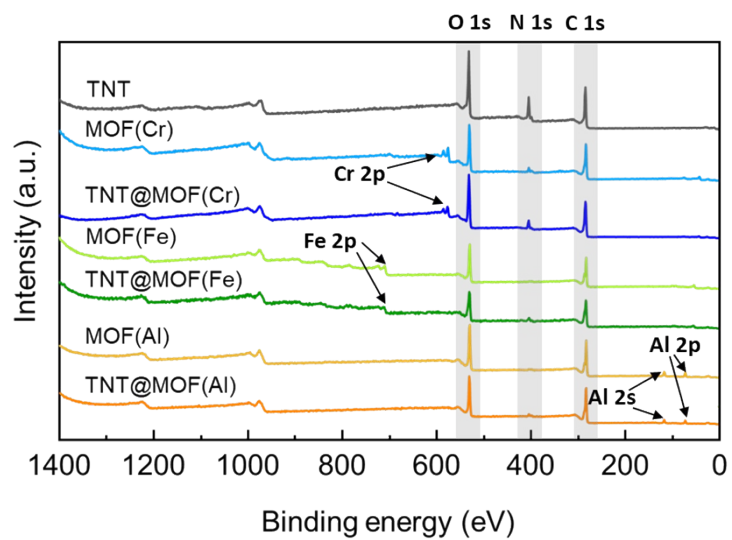
**Figure S2.** FE-SEM images of TNT.



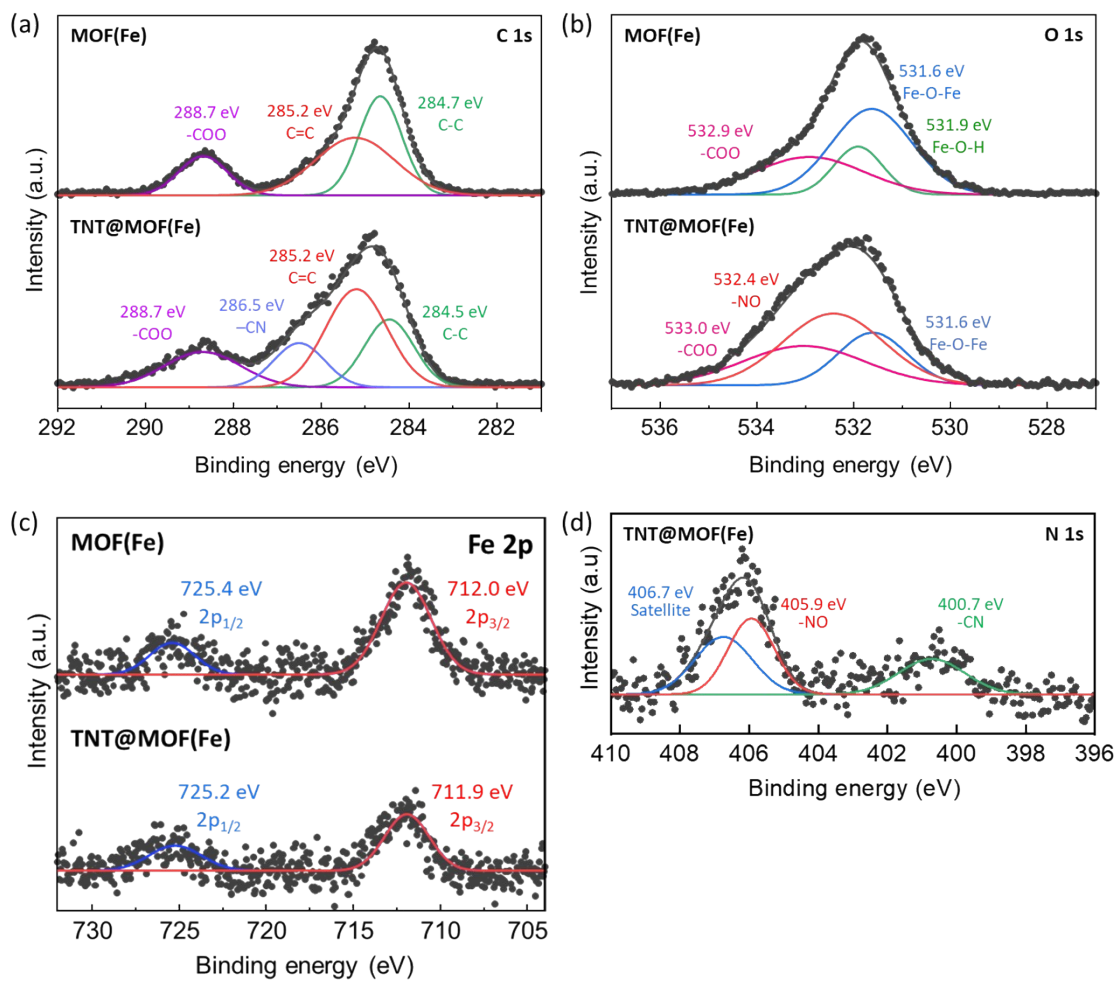
**Figure S3.** (a) IR spectra of TNT (gray) and TNT@MOFs for different metals: TNT@MOF(Cr) (blue), TNT@MOF(Fe) (green), and TNT@MOF(Al) (orange). (b) IR spectra of TNT (gray) and TNT@MOF(Cr) for different heat-treatment temperatures.



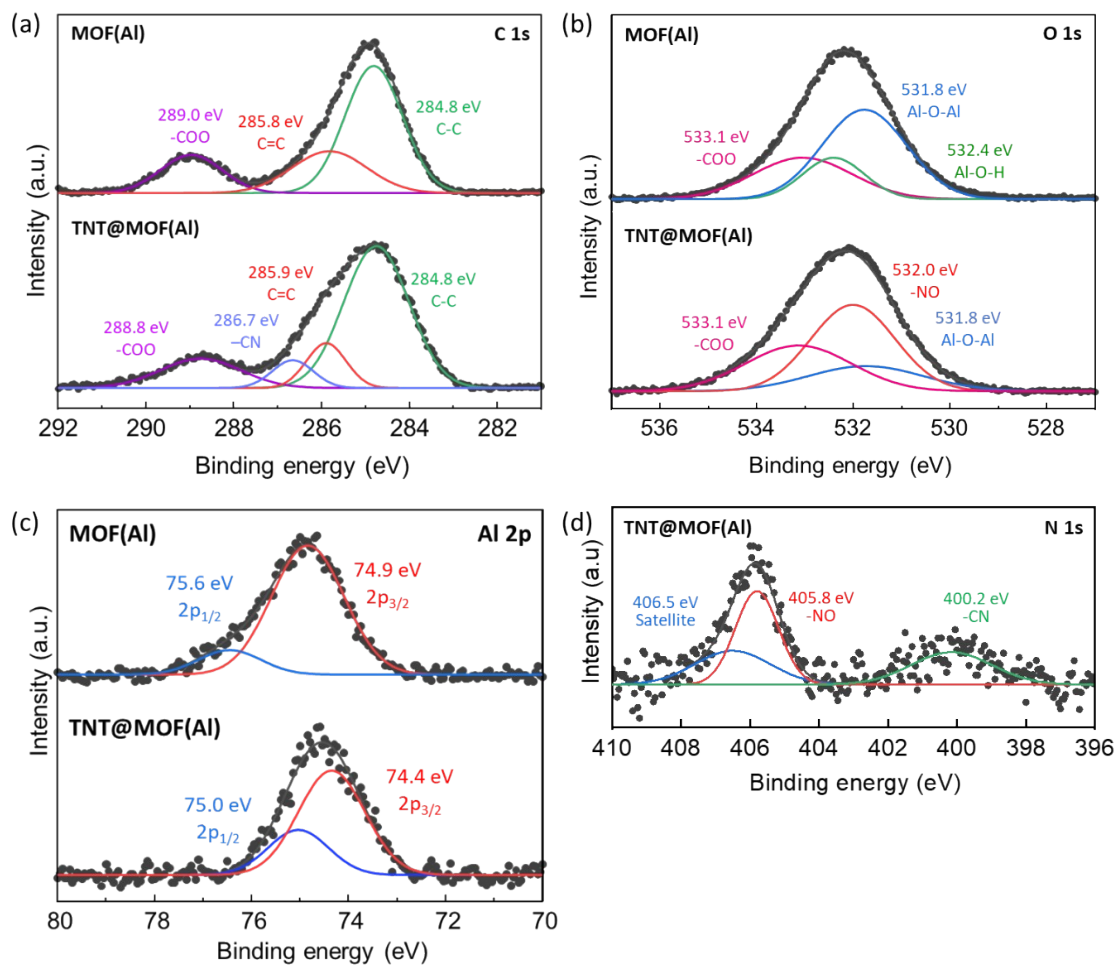
**Figure S4.** (a), (b), and (c) TGA curves of TNT (gray) and TNT@MOF from 50 °C to 600 °C and (d), (e), and (f) isothermal TGA curves of TNT (gray) and TNT@MOF at 200 °C in an N<sub>2</sub> atmosphere at a heating rate of 5 °C/min.



**Figure S5.** XPS full spectra of TNT (gray), MOF(Cr) (blue), MOF(Fe) (green), and MOF(Al) (orange) before and after TNT confinement.

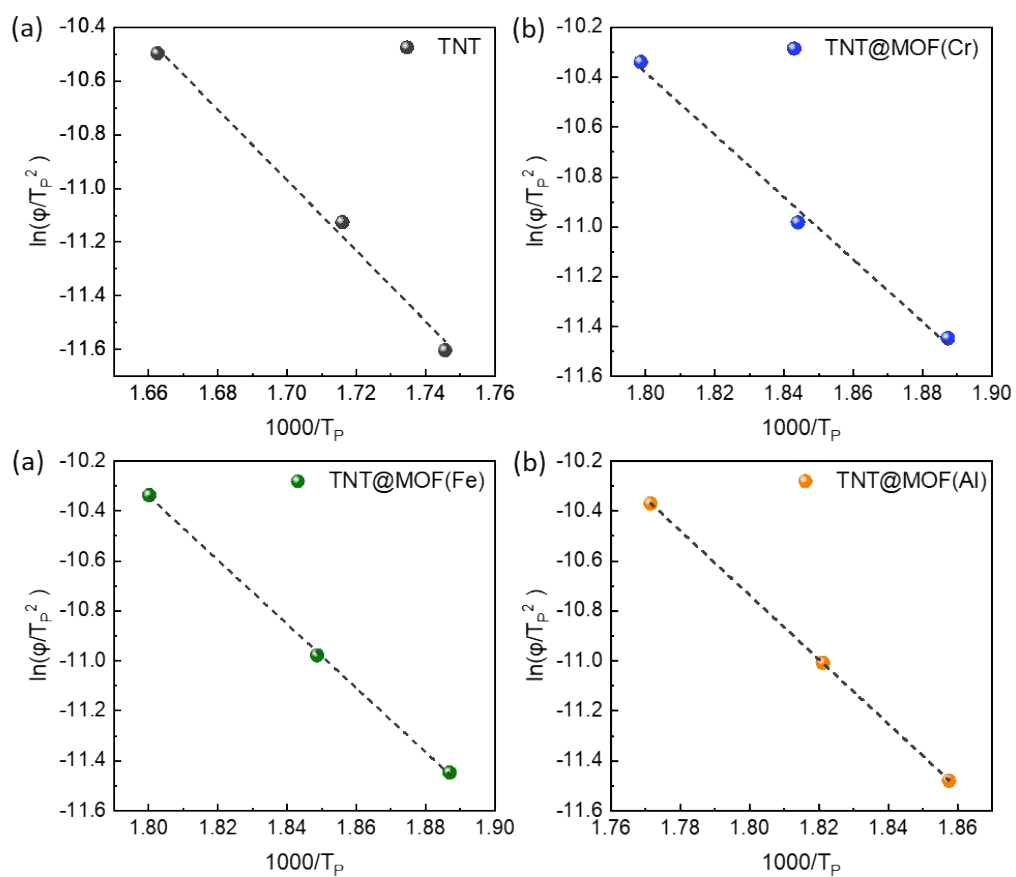


**Figure S6.** XPS spectra of MOF(Fe) and TNT@MOF(Fe) for (a) C 1s, (b) O 1s, (c) Fe 2p, and (d) N 1s.



**Figure S7.** XPS spectra of MOF(Al) and TNT@MOF(Fe) for (a) C 1s, (b) O 1s, (c) Al 2p, and (d) N 1s.





**Figure S8.** Plots of  $\ln(\phi/TP^2)$  versus reciprocal peak temperature  $1000/TP$  for (a) TNT, (b) TNT@MOF(Cr), (c) TNT@MOF(Fe), and (d) TNT@MOF(Al).

**Table S1.** Comparison of surface area and pore volume of MOFs before and after TNT confinement and pore utilization, and TNT composition.

| Porous materials                        | Surface area [m <sup>2</sup> /g] |                   | Pore utilization [%] | TNT composition [wt.%] |
|-----------------------------------------|----------------------------------|-------------------|----------------------|------------------------|
|                                         | Pore volume [cm <sup>3</sup> /g] |                   |                      |                        |
|                                         | Before confinement               | After confinement |                      |                        |
| MOF(Cr)                                 | 2518                             | -                 | 100                  | 72                     |
|                                         | 1.56                             |                   |                      |                        |
| MOF(Fe)                                 | 1608                             | -                 | 100                  | 62                     |
|                                         | 1.00                             |                   |                      |                        |
| MOF(Al)                                 | 1290                             | -                 | 100                  | 50                     |
|                                         | 0.61                             |                   |                      |                        |
| Density of TNT = 1.63 g/cm <sup>3</sup> |                                  |                   |                      |                        |

**Table S2.** Composition of TNT and MOFs before and after confinement of TNT via elemental analysis (EA) and calculations.

Unit: %

| Sample      |                       | C    | O    | N    | H   | residual |
|-------------|-----------------------|------|------|------|-----|----------|
| TNT         | Analytical value      | 39.1 | 40.1 | 18.6 | 2.3 | -        |
|             | Theoretical value [a] | 37.0 | 42.3 | 18.5 | 2.2 | -        |
| TNT@MOF(Cr) | Analytical value      | 37.5 | 32.5 | 10.3 | 2.3 | 17.5     |
|             | Theoretical value     | 37.6 | 40.2 | 14.4 | 2.2 | 6.7      |
| TNT@MOF(Fe) | Analytical value      | 35.7 | 36.9 | 9.4  | 2.1 | 16.0     |
|             | Theoretical value     | 38.4 | 39.9 | 11.5 | 2.2 | 8.0      |
| TNT@MOF(Al) | Analytical value      | 35.4 | 33.4 | 9.5  | 2.3 | 19.4     |
|             | Theoretical value     | 37.7 | 43.8 | 9.3  | 2.1 | 7.2      |

[a] Values calculated from the TNT and MOFs compositions via EA and ratio of TNT and MOFs inside the samples.

**Table S3.** DSC measurements of onset, endset, and maximum temperature and activation energy values of TNT, TNT@MOF(Cr), TNT@MOF(Fe), and TNT@MOF(Al)

| Sample      | Heating rate<br>[K/min] | Temperature of exothermic peak [K] |                     |                      | Activation energy<br>[kJ/mol] |
|-------------|-------------------------|------------------------------------|---------------------|----------------------|-------------------------------|
|             |                         | T <sub>onset</sub>                 | T <sub>endset</sub> | T <sub>maximum</sub> |                               |
| TNT         | 3                       | 567                                | 578                 | 573                  | 109.11                        |
|             | 5                       | 576                                | 590                 | 583                  |                               |
|             | 10                      | 594                                | 613                 | 602                  |                               |
| TNT@MOF(Cr) | 3                       | 501                                | 642                 | 530                  | 103.86                        |
|             | 5                       | 511                                | 654                 | 542                  |                               |
|             | 10                      | 524                                | 672                 | 556                  |                               |
| TNT@MOF(Fe) | 3                       | 511                                | 593                 | 530                  | 106.46                        |
|             | 5                       | 511                                | 611                 | 541                  |                               |
|             | 10                      | 521                                | 634                 | 556                  |                               |
| TNT@MOF(Al) | 3                       | 509                                | 630                 | 538                  | 107.13                        |
|             | 5                       | 512                                | 648                 | 549                  |                               |
|             | 10                      | 533                                | 660                 | 565                  |                               |