

## Optimized energetic HNTO/AN co-crystal and its thermal decomposition kinetics in presence of energetic coordination nanomaterial-based on functionalized graphene oxide and cobalt

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### SUPPLEMENTARY MATERIALS

#### 1. Preparation of catalysts

##### 1.1. Preparation procedure of GO-T

In a beaker, 200 mg of GO was added to 200 mL of distilled water under high power ultrasonication to form a fully dispersed form of aqueous solution. A mixture containing 50 mg of 1-ethyl-3-(3-dimethylamino)propyl)carbodiimide (EDC) and 40 mg N-hydroxysuccinimide (NHS) was added to the dispersed GO. The final prepared mixture is left to react under moderate stirring for at least one hour until the formation of a dark grey agglomeration. After that, 2 g of triaminoguanidine nitrate (T·HNO<sub>3</sub>) was added to the resultant homogenous mixture under vigorous stirring at around 75 °C for 4 h. Black flocculants were progressively precipitated, filtered and rinsed with copious amount of distilled water. The presence of HNO<sub>3</sub> acid in the liquid solution has decrease the pH value to around 2.0–4.0. Subsequently, NaHCO<sub>3</sub> was added dropwise to increase the pH of the solution. The resultant product (1.4 g) corresponds to the exfoliated and decorated GO with T via a cross-linking of –CO–NH–(GO–T).

##### 1.2. Preparation procedure of T-Co

Under mechanical stirring, 1 mmol of T·NH<sub>3</sub> was dispersed in 20 mL of distilled water for 10 min at room temperature. Certain amount of cobalt perchlorate hexahydrate (457.41 mg) is added drop wise to the solution. After that, the temperature of the solution was raised to 80 °C and was allowed to react at least for 2 h. The obtained product was then neutralized by sodium

bicarbonate until filtrates becoming neutral. The black precipitate was filtered and washed with distilled water for several times.

### 1.3. Preparation procedure of GO-T-Co-T

A solution of one mmol of T-Co was added to 20 mL of distilled water containing 1mmol of GO-T. The mixture reacts for 4 h at a controlled temperature of 75 °C. The precipitate is then filtrated and rinsed repeatedly with water. The produced layered hybrid crystals correspond to GO-T-Co-T.

## 2. Characterizations of the catalysts

The SEM micrographs of the used catalysts are illustrated in Fig. S1. Further, based on EDX results depicted in Fig. S2, the atomic cobalt content in T-Co and GO-T-Co-T.

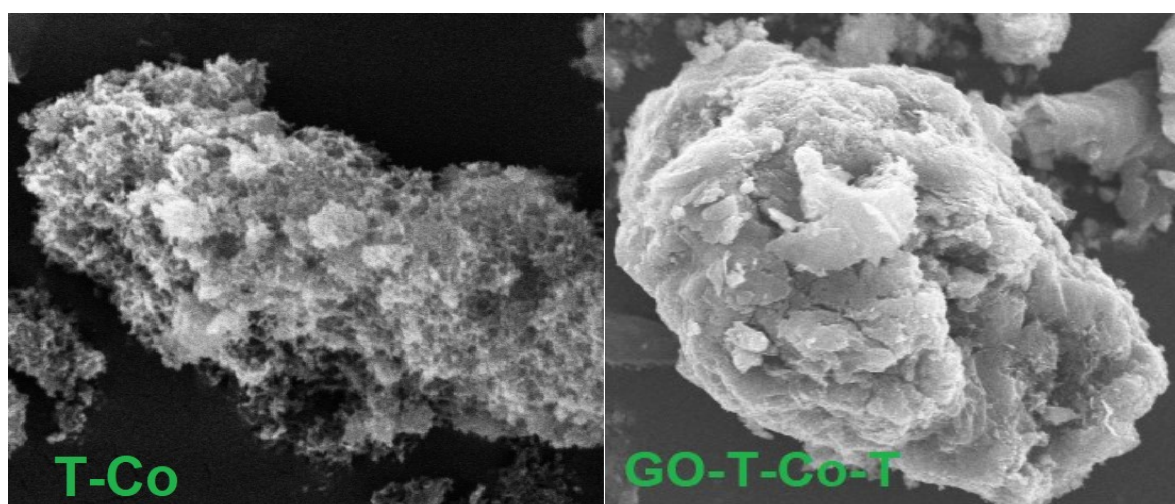
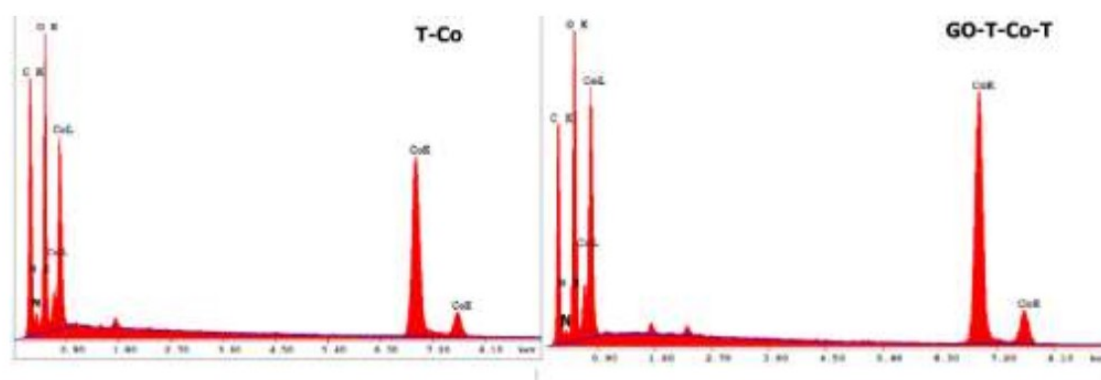
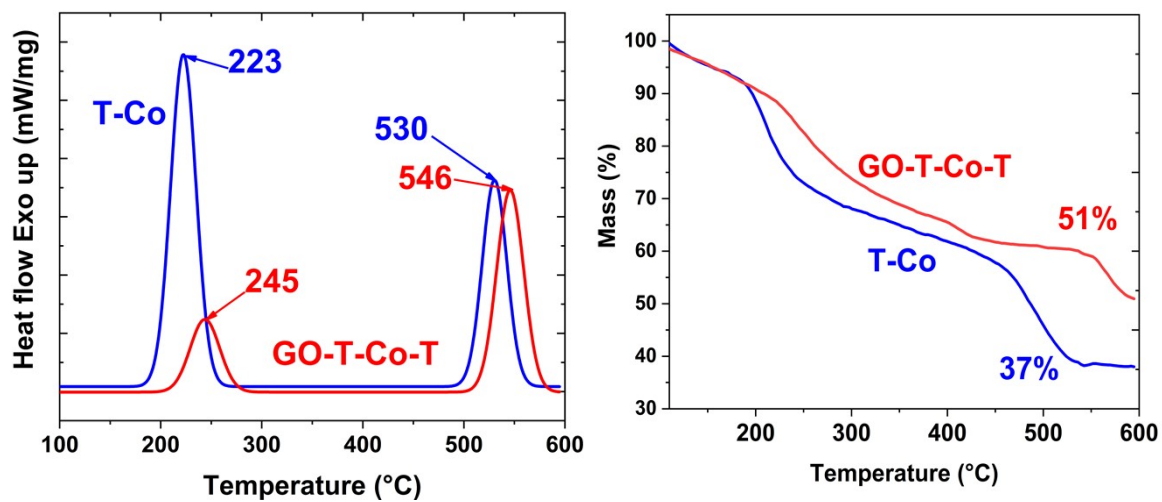


Figure S1



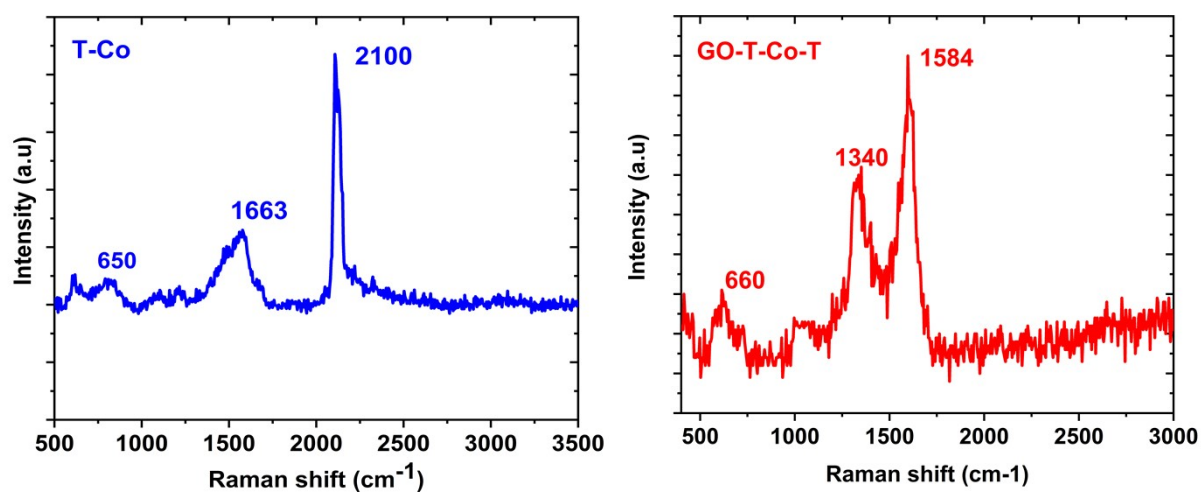
**Figure S2**

The thermal properties of the used catalysts have been determined by using DSC/TGA methods at a heating rate of 10 °C/min (Fig. S3).



**Figure S3**

Raman spectra of the prepared catalysts as well as their FTIR spectra are illustrated in Fig.S4 and Fig.S5, respectively.



**Figure S4**

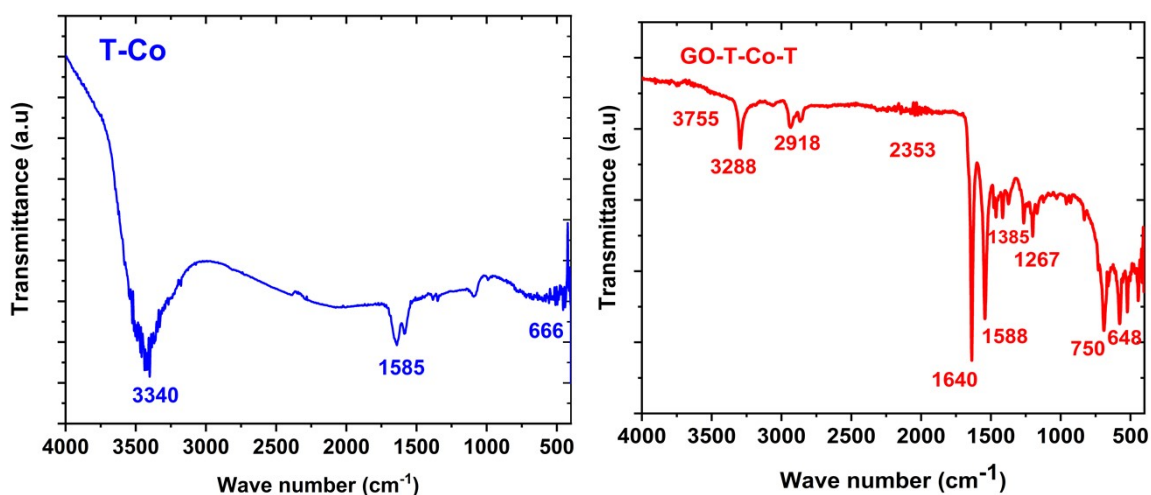


Figure S5

### 3. FTIR and XRD of HNTO and AN

Fig. S6 shows the PXRD patterns, including the raw HNTO and AN. Comparing the XRD results of the co-crystal shown in Fig.5 with that of pure compound, a set of diffraction peaks that belong to HNTO and AN disappears and numerous new diffraction peaks appear. The peaks that have been disappeared are the peaks at 27.6°, 16.4°, 14.4°, 13.2°, and 8.2° for HNTO and 54.3°, 35.6°, 24.9°, 23.8°, 19.5° and 15.4° for AN (JSPDS file no. 47-0867). The cocrystal has a unique X-ray diffraction pattern, which identifies it as a new material rather than a simple mixture.

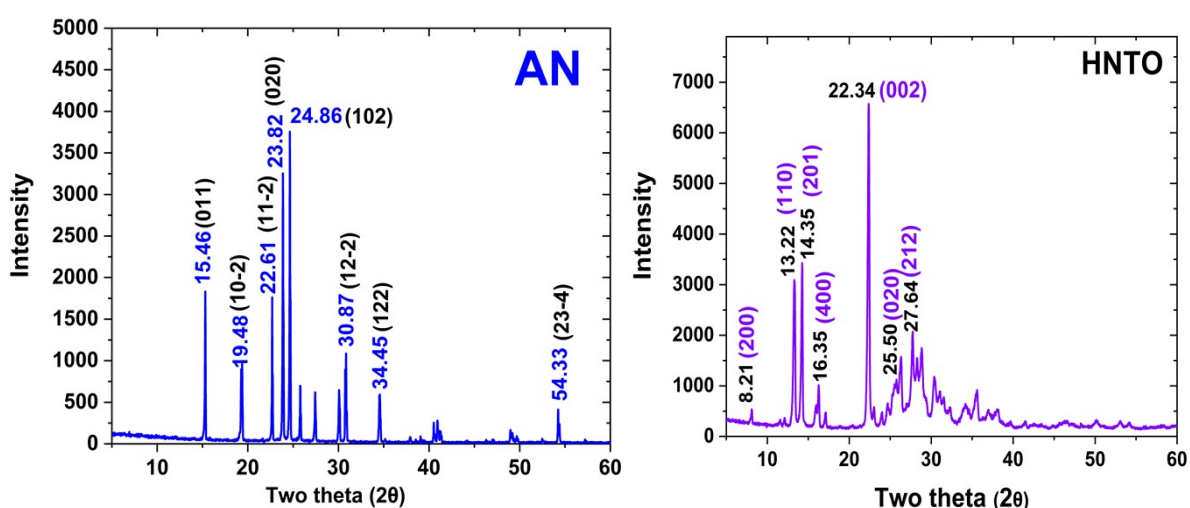
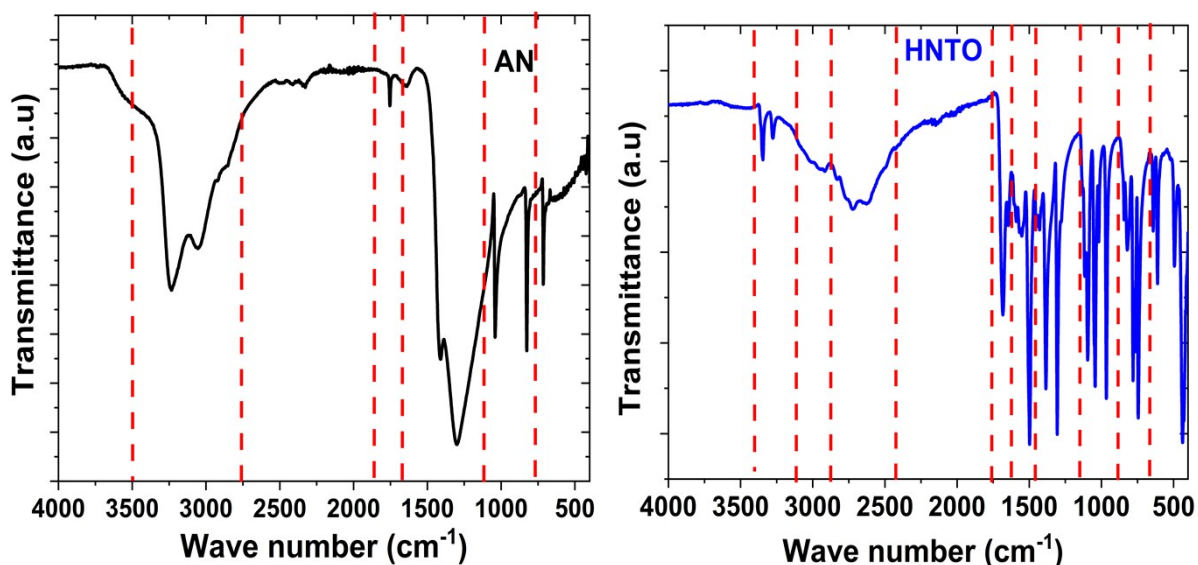


Figure S6.



**Figure S7**

In addition, Fig. S7. depicts the IR spectra of raw HNTO. From this figure, we can see that the raw materials have similar IR spectra with the cocystal (Fig.5), but they still have differences more or less. It can be established from the chart that all main vibrational bonds of HNTO and AN in the region of 2500-3400  $\text{cm}^{-1}$  are shown on the cocystal infrared spectroscopy spectra, while most vibration peaks have a shift at least by 15  $\text{cm}^{-1}$ . Furthermore, new IR absorption peaks at 2425, 1291, 1256 and 563  $\text{cm}^{-1}$  were observed after formation of the cocystal. Others have been reduced or even disappear such as at 2324  $\text{cm}^{-1}$ , 1759  $\text{cm}^{-1}$ , and 820  $\text{cm}^{-1}$  for AN and at 2724  $\text{cm}^{-1}$ , 1305  $\text{cm}^{-1}$ , and 812  $\text{cm}^{-1}$  for HNTO. The appearance of the new IR peaks may be the result of the cocystal formation via intermolecular interactions between the two raw compounds, while the red-shift of these peaks indicates that the reaction of AN with HNTO reduces the electron density of the carbonyl and nitril groups.