# Supporting Information

## Constructing Graphene-like Structure to Lower Friction Sensitivity: Ag(I) Complexes Based on Furan-2,5-dicarbohydrazide

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# Experimental Section

**Caution!**

In the research process, the chemicals we use, including raw materials and target compounds, are potentially dangerous. Although we didn't encounter any danger in the process of synthesis and characterization, we still strongly recommend taking necessary protective measures before approaching these items, including using the specified experimental clothes, gloves, masks and baffles. All operations must be carried out in the fume hood.

**Materials and Equipment**

During the experiment, the reagents (analytical grade) used were purchased from Aladdin and Azov and used without further purification. Single crystal X-ray diffraction data was collected by using Rigaku supernova single X-ray diffractometer area detector ($Mo_{K\alpha'}$, 0.71073 Å). Powder X-ray diffraction (PXRD) data of the product was tested using a Bruker D8 ADVANCE X-ray powder diffractometer ($Cu_{K\alpha'}$, 1.5418 Å). The thermal behavior of the compound was analyzed by differential scanning calorimeter (TGA/DSC2, METTLER TOLEDO STAR $^{e}$ system), with the heating rate was 5 $K \cdot min^{-1}$, and the gas atmosphere was $N_2$. Infrared (IR) spectra were measured on a Nicolet Is10 spectrometer (Equipped with KBr discs) with a measurement range of 4000 - 400 $cm^{-1}$ . Elemental analyses (C,H,N or C,H,N,S) were carried out on an elemental analyzer (Vario EL Cube, Germany). The mechanical sensitivities (including impact sensitivity and friction sensitivity) of the material were determined by the standard step method of the drop weight device with a BAM DFH-10 device with a weight drop of 5 kg. The constant pressure reaction heat is measured by High Pressore Oxygen Calorimeter (BCA@ 500), with the standard molar combustion enthalpy can be converted by the combustion equation. The experimental density is obtained by the powder densitometer test (Micromeritics AccuPyc II 1340). The laser performance test is measured by Diode Laser (Changchun laser technology co., LTD. LR-ISP-980/1~1000mW. Spectral Line width (nm): < 3, Output Power (mW): 1~1000, Beam Diameter at Aperture (mm): 5.0 x 5.0, Modulating Repetition: 100KHz TTL / 10KHz Analogue. Operating parameters: theoretical maximal output power $P_{max}$ = 30.15 W; theoretical pulse length $\tau_{max}$ = 49571 μs. wavelength $\lambda$ = 915 nm. Frequency F = 1Hz.).

**Synthesis of furan-2,5-dicarbohydrazide (FDCA, 1)**

0.05 mol (9.21 g) of 2,5-furandicarboxylic acid dimethyl ester was dissolved in 80 mL of methanol , stirring, and then 0.12 mol (7.06 g) of 85% hydroxylamine hydrate was added. The mixture was refluxed at 80℃ overnight, filtered, washed with alcohol, and dried to obtain the desired product **1** in a pale yellow powder form. Yield: 86%.

IR (KBr, ν/cm-1): 3104 (m), 1685 (m), 1624 (m), 1592 (s), 1527 (s), 1375(s), 1248 (s), 1045 (s), 996 (s), 924 (s), 839 (s), 677 (s).

MS (ESI), m/z: 183.06 [$C_6H_7N_4O_3^-$].

Elemental analysis (%) for $C_6H_8N_4O_3$ (Mr = 184.06 g mol-1): calcd. C 39.13, H 4.38, N 30.42;

found C 39.03, H 4.22, N 31.15.

$^{13}$C NMR (400 MHz, DMSO-d6), (δ: ppm): 114.6, 147.5, 157.5.

**Synthesis of Ag(FDCA)$ClO_4$ (ECPs-1)**

0.01mol (1.8 g) of **1** was suspended in aqueous solution, heated to 40℃ and dissolved by adding a small amount of acid. Drop about 0.1mol of $AgClO_4$ solution, then a large amount of white solid is produced immediately. Add $HClO_4$ drop by drop until the solid is dissolved, filter while it is hot, and let it stand and cool for 2-3 days to obtain white transparent crystal (**ECPs-1**). Yield: 78%.

IR (KBr, ν/cm-1): 3306 (m), 3106 (m), 1668 (m), 1596 (s), 1554 (s), 1299 (s), 1213 (s), 1094 (s), 1027 (s), 960 (s), 844 (s), 765 (s).

Elemental analysis (%) for $C_6H_8N_4O_7AgCl$ (Mr = 391.47 g mol-1): calcd. C 18.41, H 2.06, N 14.31; found C 18.27, H 1.91, N 14.55.

**Oxygen bomb calorimetry**

The constant pressure reaction heat ($\Delta_C U$) of **ECPs-1** was measured by an oxygen bomb calorimeter, and the average value was obtained by three measurements independently. The standard molar combustion enthalpy ($\Delta_C H^\theta_m$) can be obtained from the constant pressure reaction heat ($\Delta_C U$) according to the equation (**1**). According to the principle of Hess' law, the complete combustion reaction equation of **ECPs-1** were shown in equation (**2**), and the standard molar generation enthalpy ($\Delta_f H^\theta_m$) can be obtained based on the formulas (**2**) and (**3**) [ $\Delta_f H^\theta_m$: $CO_2$(g): -393.51 kJ mol$^{-1}$; $H_2O$(l): -285.83 kJ mol$^{-1}$; AgCl(s): -127.04 kJ mol$^{-1}$]. The final experimental results showed that the combustion heats of **ECPs-1** is 8207 J g$^{-1}$.

$$\Delta cH^\theta m = \Delta cU + \Delta nRT \quad (1)$$

$\Delta_n$ = $n_g$(products)-$n_g$(reactants), ($n_g$ is the sum of the total moles of gas in the product or reactant, $R$ = 8.314 J mol$^{-1}$ K$^{-1}$, $T$ = 298.15 K)

$$C_6H_8N_4O_7AgCl(s) + {}^9/_2 O_2(g) = 6CO_2(g) + 4H_2O(l) + 2N_2(g) + AgCl(s) \quad (2)$$

$$\Delta_f H^\theta m(compound) = \sum \Delta_f H^\theta m(products) - \Delta_c H^\theta m(compound) \quad (3)$$

**Theoretical simulation based on K-J equations**

The constant pressure reaction heat ($\Delta_C U$) of compounds were measured by an oxygen bomb calorimeter, Detonation speed (D) and explosion pressure (P) are the main indicators for measuring energetic materials. The various detonation characteristics were predicted by using the modified Kamlet-Jacbos (K-J) equations ( eq 5-7) which is a commonly used equation for predicting the detonation velocity and pressure of high energy materials.

$$C_6H_8N_4O_7AgCl(s) = 3CO(g) + 3C(s) + 4H_2O(g) + 2N_2(g) + AgCl(s) \quad (4)$$

$$D = 1.01(NM^{1/2}Q^{1/2})^{1/2}(1 + 1.30\rho) \quad (5)$$

$$P = 1.55\rho^2 NM^{1/2}Q^{1/2} \quad (6)$$

$$Q = \frac{-[\Delta H_f(\text{detonation production}) - \Delta H_f(\text{explosive})]}{\text{formulaweightof explosive}} \quad (7)$$

D: detonation velocity, km $s^{-1}$); P: detonation pressure, GPa; ρ: density, g $cm^{-3}$; $\Delta H_f$: heat of formation, kJ $mol^{-1}$); Q: heat of detonation, J $g^{-1}$); N: moles of detonation gases per gram of explosive, mol $g^{-1}$); M: average molecular weight of gases, g $mol^{-1}$).

**Hot needle (HN) tests**

Approximately 20 mg of the compound was dispersed on the operating table in a powdered state. The tiny iron needle is heated, and then slowly approached the compound, while recording the deflagration process of the compound with a high-speed camera.

**Detonation initiation**

The test device used to breakdown of the lead plate, the material inside can be divided into two parts: the first part is filled with compound **ECPs-1** (100 mg, pressure of fixation is 25 MPa); the second component is RDX (400 mg, charge pressure is 40 MPa). The lead plate has a thickness of 5 mm.

**Laser performance test**

Weigh 10 mg samples (pressure of fixation is 20 MPa), a total of 5 parts, and place them in sample tubes. Use a semiconductor laser to trigger the sample. Determine the minimum trigger energy by adjusting the action time and power. Take the average value as the final test value.

# Supplementary Figures S1 – S6

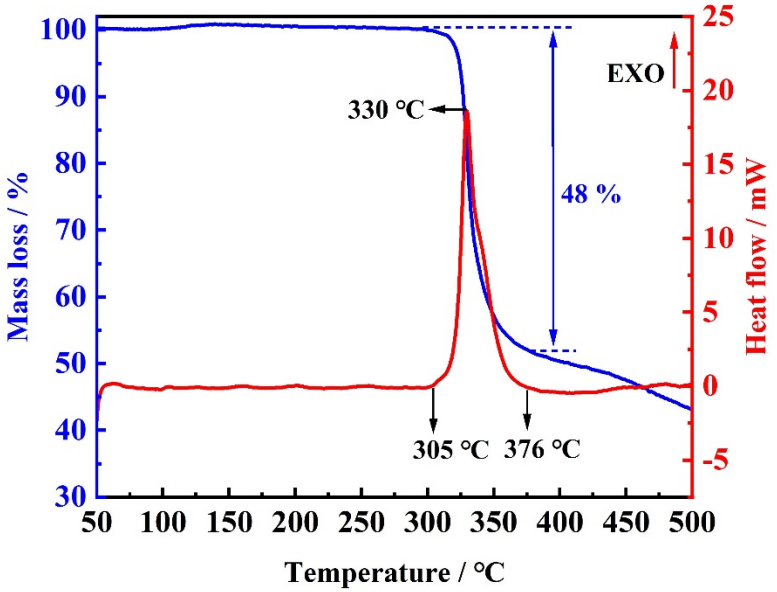


**Figure S1 DSC-TG** of **Ag(FDCA)ClO$_4$**.

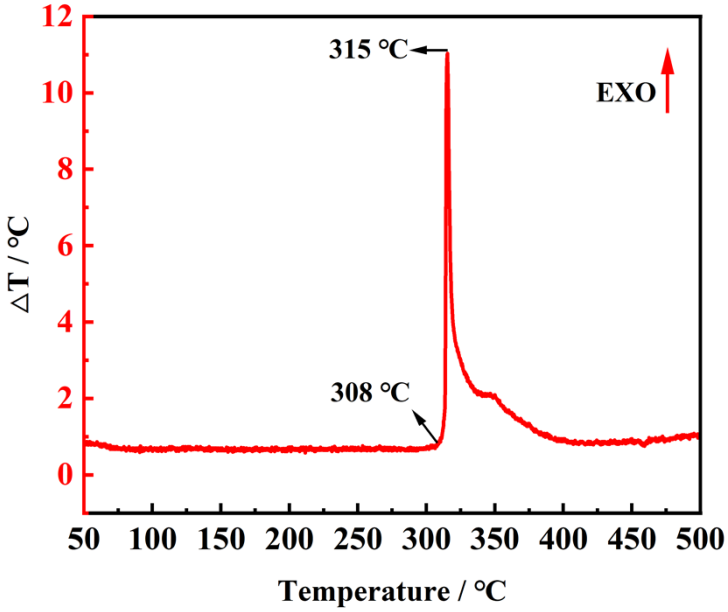


**Figure S2 DTA** of **Ag(FDCA)ClO$_4$**.

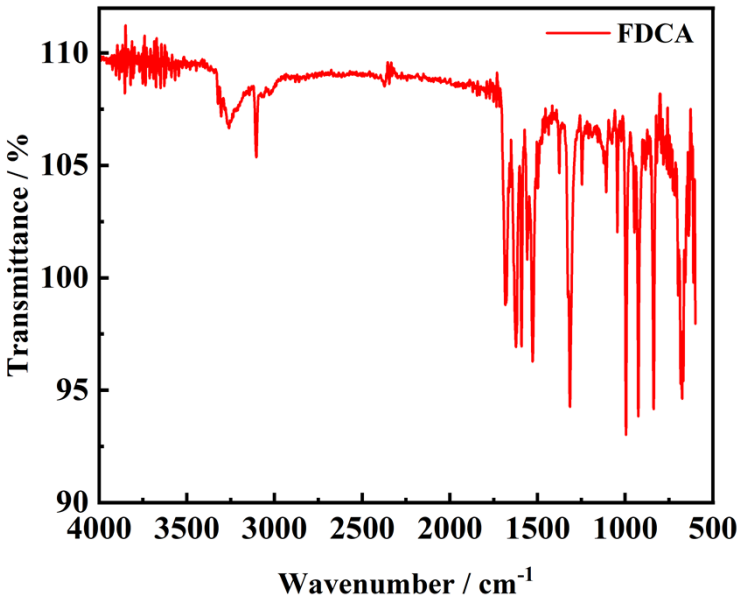


**Figure S3 IR** of **FDCA**

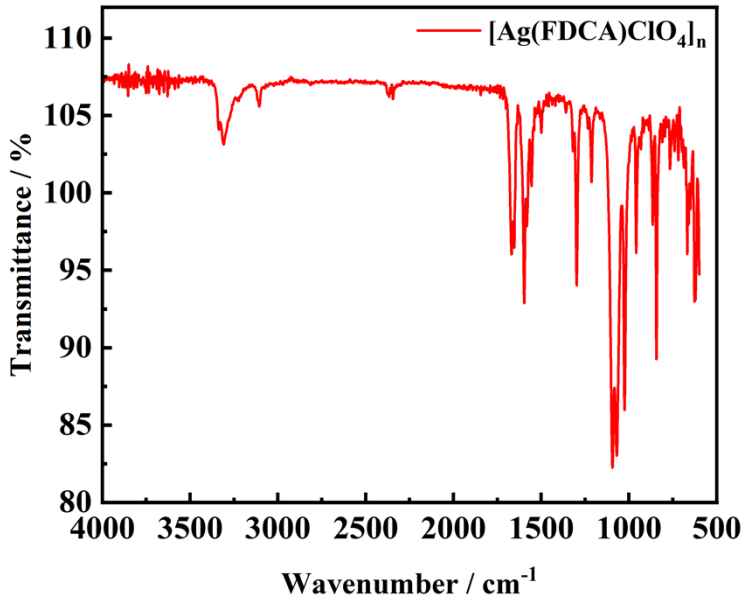


**Figure S4 IR** of **Ag(FDCA)$ClO_4$**.

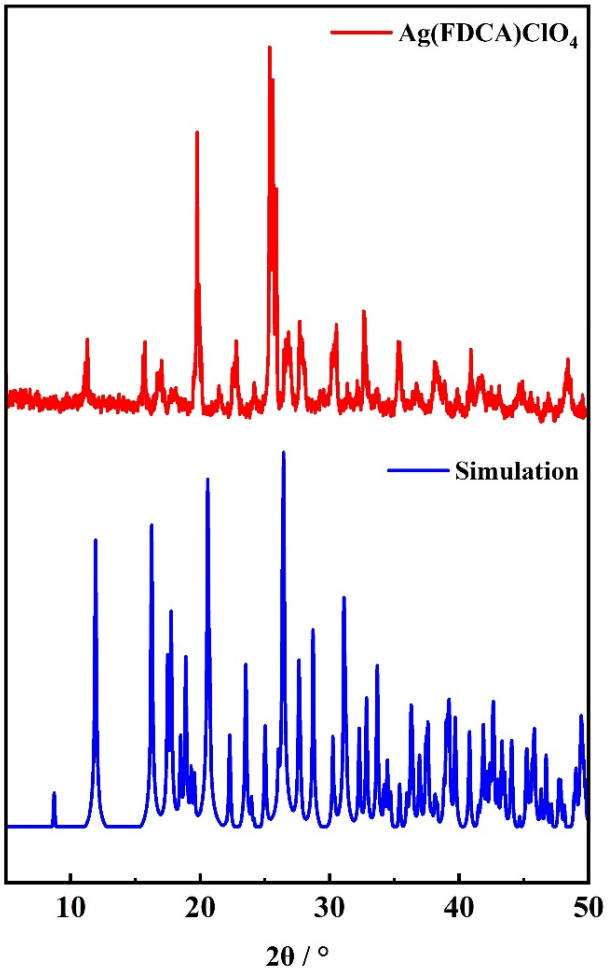


**Figure S5 P-XRD** of **Ag(FDCA)$ClO_4$**.

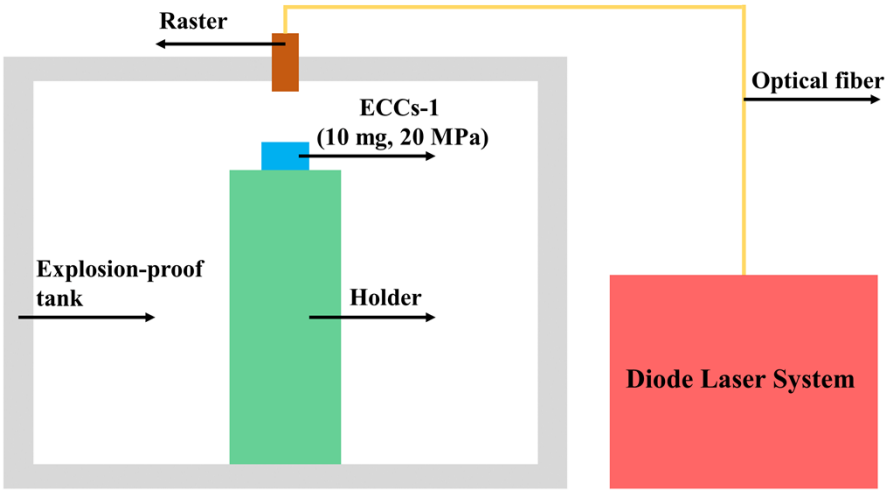


**Figure S6** Illustration of setup of Laser Initiation Tests.

# Supplementary Table S1

**Table S1.** Crystallographic data for **Ag(FDCA)ClO$_4$**

| | |
|---|---|
| Formula | $C_6H_8N_4O_7ClAg$ |
| Temperature [K] | 298.15 |
| $M_w$[g mol$^{-1}$] | 391.474 |
| Crystal size [mm$^3$] | 0.3 x 0.1 x 0.07 |
| Crystal system | Monoclinic |
| Space group | $P2_1/m$ |
| unit cell dimensions | $a$[Å]= 5.0231(5), $b$[Å]= 10.8971(9), $c$[Å]= 10.2026(9) |
| | $\alpha$[°]= 90, $\beta$[°]= 96.600(3), $\gamma$[°]= 90 |
| $V$[[Å$^3$] | 554.76(9) |
| $Z$ | 2 |
| $\rho_{calc}$[g cm$^{-3}$] | 2.344 |
| $\mu$[mm$^{-1}$] | 2.097 |
| $F$(000) | 382.8 |
| 2$\theta$ range[$^o$] | 5.48 - 50.04 |
| Reflections collected | 3332 |
| Index ranges | -6 ≤ h ≤ 4, -14 ≤ k ≤ 13, -12 ≤ l ≤ 13 |
| $R_{int}$ | 0.0396 |
| Data/restraints/parameters | 1029/18/102 |
| Final R index [$I > 2\sigma(I)$] | R1 = 0.0450, wR2 = 0.1052 |
| Final $R$ index [all data] | R1 = 0.0555, wR2 = 0.1105 |
| GOF on F$^2$ | 1.038 |
| CCDC | 2257652 |