Supporting information

for

Desensitization of Spherical CL-20 Composites by Embedding Insensitive Nanosized Energetic Crystals

Zhi-Hua Xue[1], Ruixuan Xu[1], Jianheng Qin[1], Zikangping Wang[1], Yu Liu[2], Qi-Long Yan[1*]

1. National Key Laboratory of Solid Rocket Propulsion, Northwestern Polytechnical University, Xi'an 710072, China.

2. Institute of Chemical Materials, China Academy of Engineering Physics, Mianyang 621900, China

Corresponding E-mail: qilongyan@nwpu.edu.cn

Contents

S1 The Preparation and characterizations of target products

S1.1 Materials and Reagents

CL-20, LLM-105 and FOX-7 were commercially available without the need for further purification (purity > 99.5%). Dopamine and (hydroxymethyl) aminomethane (Tris) were obtained from Sigma-Aldrich and used as received.The analytical pure ethyl acetate, acetone, absolute ethyl alcohol and deionized water used in the present study were commercially available and used as they were without further purification.

S1.2 Experimental

***Ball milling processing*:** Place 10 g of LLM-105 (FOX-7) raw material, 250 g of high-purity ZrO_2 grinding balls (ϕ=0.1 mm, 1 mm), 25 ml of ethanol, and 25 ml of distilled water into a ZrO_2 grinding jar (with a volume of approximately 250 ml) and seal it. Install the ZrO_2 grinding jar, set the rotational speed to 550 rpm, and grind for 8 hours before extracting the moist powder. Separate the balls from the powder and freeze-dry them to obtain nano-sized LLM-105 and FOX-7 crystals.

***Coating modification*:** 0.18 g dopamine-HCl was dissolved in 150 ml of TRIS buffer (pH = 8.5), followed by the addition of 3 g LLM-105 (FOX-7). The solution was stirred for 2 h, and the products were filtered and washed with distilled water several times.

***Preparation of co-particle*:** Firstly, the raw material CL-20 was dissolved in ethyl acetate. Secondly, with magnetic stirring and ultrasonic waves, a certain amount of nLLM-105@PDA (nFOX-7@PDA) was added to the solution mentioned above to create a homogeneous suspension. Thirdly, the nitrogen flow and feed rate were set to 60 °C, 350 and 4.5 $mL \cdot min^{-1}$, respectively. Finally, the suspension was rapidly dried via spray-drying, resulting in the co-LLM-105_P/CL-20 and co-FOX-7_P/CL-20 co-particles.

According to the mentioned co-LLM-$105_{P10\%}$/CL-20 (co-FOX-$7_{P10\%}$/CL-20) ratio, co-LLM-$105_{10\%}$/CL-20 (co-FOX-$7_{10\%}$/CL-20) was obtained by spray-drying a mixture of non-surface functionalized nLLM-105 (nFOX-7) and CL-20. CL-20 and nLLM-105@PDA (nFOX-7@PDA) were placed in a mortar. Ethanol was then added as an auxiliary solvent, and the m-LLM-$105_{P10\%}$/CL-20 and m-FOX-$7_{P10\%}$/CL-20 samples were obtained by grinding the mixture physically. The shells of co-LLM-$105_{P10\%}$/CL-20 and co-FOX-$7_{P10\%}$/CL-20 co-particles were dissolved with ethyl acetate to obtain their internal structures.

S1.2 Characterizations

Structures and morphologies: Structures and morphologies: The morphologies of the specimens were recorded by using a scanning electron microscope (SEM; SIGMA HD, Zeiss). The surface chemistry was analyzed using X-ray photoelectron spectroscopy (XPS; Thermo Scientific ESCALAB Xi+) equipped with monochromatic Al Kα radiation (1486.68 eV). Data processing and peak fitting were carried out using the XPSPeak4.1 software. Background subtraction was performed using the Shirley method, and the peaks of the elements were fitted with a Gaussian-Lorentzian mixed function, with constraints applied to the peak positions and full width at half maximum (FWHM). The fitted peak areas were quantitatively converted based on sensitivity factors to obtain the relative concentrations of the elements. Raman measurements were performed with an Raman spectrometer (Thermo DXR2xi). Powder X-ray diffraction (XRD) patterns were recorded on a Smart Lab 9KW with a Cu Kα radiation; the voltage and current applied were 40 kV and 150

mA, respectively. The data were collected from 5° to 90° in 2θ, with an increment of 0.01° and a scan speed of 10 s per step. Fourier transform infrared (FT-IR) spectra were taken in Fourier transform infrared spectroscopy (FTIR, Bruker, US) with a scanning range from 650 to 4500 cm^{-1}. The heat of combustion was measured in a calorimetry bomb filled with 3 MPa of pure oxygen, with a sample mass of about 1.0 gram for each test. Each content was calculated through their average value. The mechanical sensitivity of the sample was determined by the material contact characteristic tester (Adision, FST 20) and the material impact characteristic tester (Adision, BFH 20).

Performances: The crystal density was measured by a densitometer with a chamber size of 5 ml, filled with helium at a pressure of 17 psi, where the sample mass for each test is about 1.0 gram. The heat of combustion was measured in a calorimetry bomb filled with 3 MPa of pure Ar, with a sample mass of about 1.0 gram for each test. Thermal analysis was performed on a simultaneous TG-DSC instrument (NETZSCH, STA-692 F5). The samples were heated from 40 °C to 400 °C at a heating rate of 2.5, 5 and 7.5 °C min^{-1} under Nitrogen atmosphere.

S2 The morphology and structural characterization of nLLM-105@PDA and nFOX-7@PDA

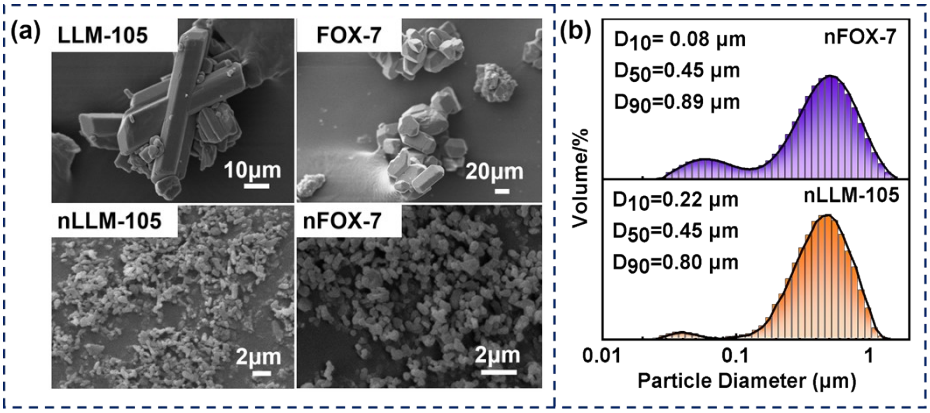

Figure S1 SEM images (a) of and the particle size distribution curve (b) of nLLM-105 and nFOX-7

The morphology of LLM-105 and FOX-7 particles was characterized using scanning electron microscopy (SEM) characterization after ball-milling (**Figure** S1a). LLM-105 particles exhibited a needle-like shape while displaying significant defects. The average particle size of LLM-105 was approximately 50 μm. The raw FOX-7 demonstrated heterogeneous shapes, marked by a wide variance in particle size, together with roughened surfaces and edges. After the milling process, raw LLM-105 and FOX-7 were effectively pulverized into highly fragmented particles of consistent size and morphology. The size distribution curves of nLLM-105 and nFOX-7 are depicted in **Figure** S1b, revealing a median diameter (d_{50}) of 450 nm, which denotes that half of the particle population exhibits diameters less than 450 nm. **Figure** S2a reveals that the milled LLM-105 and FOX-7 phases do not undergo any changes throughout the pulverization process. Furthermore, the X-ray Photoelectron Spectroscopy (XPS) results (**Figure** S2b) confirmed that the nanoscale LLM-105 and FOX-7 samples remained uncontaminated during ball-milling. **Figure** S3 in the Supplementary Material provides photographs of the nLLM-105 and nFOX-7 samples with a polydopamine (PDA) coating. The PDA coating turned the samples into a dark green color. The XPS tests enable the detection of changes in the electron binding energy of elements on the surface of nLLM-105 and nFOX-7 due to the PDA coating.

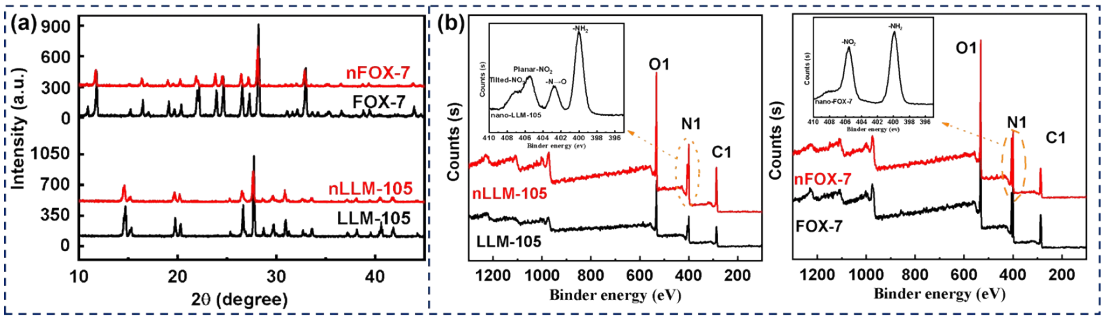

Figure S2 The XRD pattern (a) and XPS pattern (b) of nLLM-105 and nFOX-7

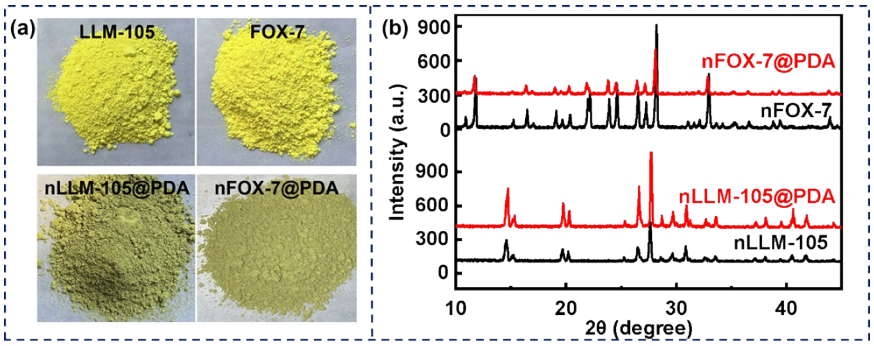

Figure S3 The appearance picture (a) and XRD pattern (b) for nLLM-105@PDA and nFOX-7@PDA

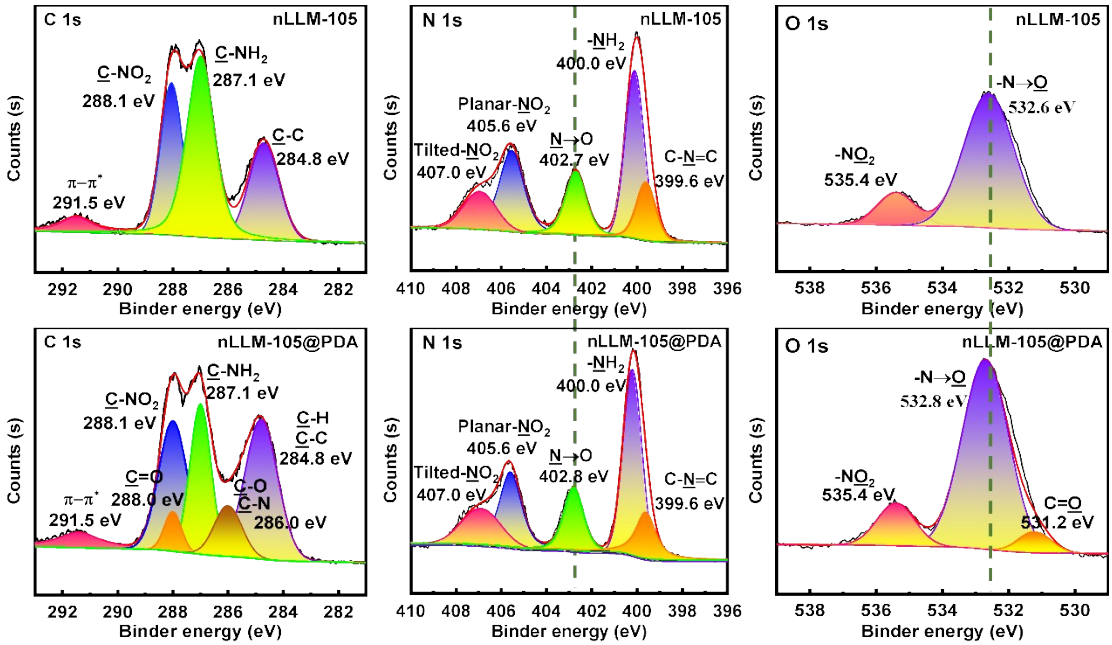

Figure S4 The XPS pattern for nLLM-105 and nLLM-105@PDA

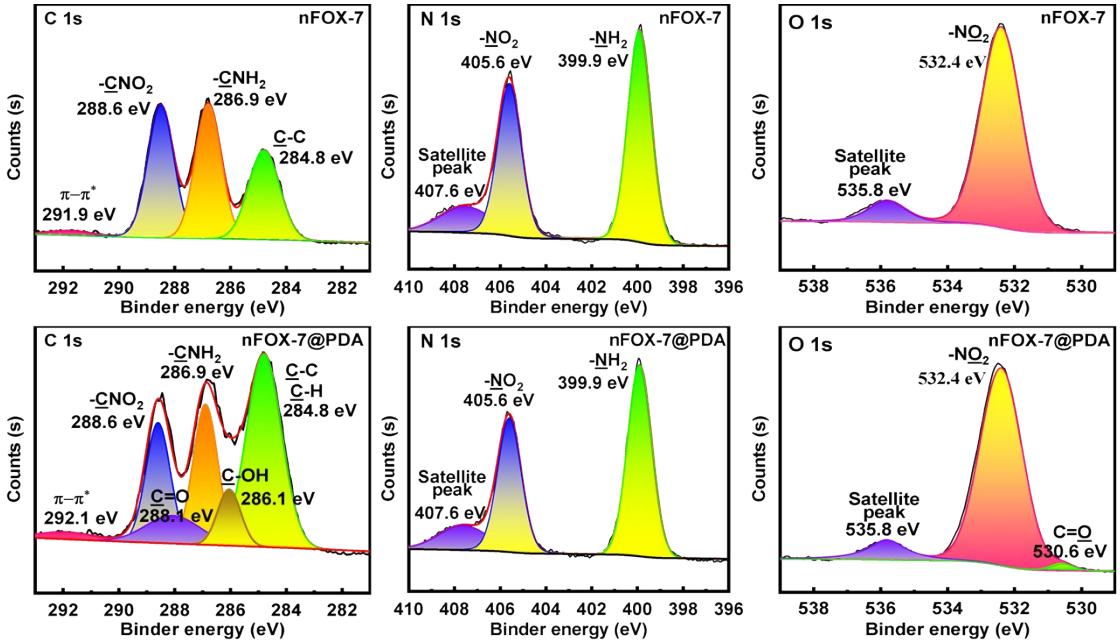

Figure S5 The XPS pattern for nFOX-7 and nFOX@PDA

S3 The morphology of co-particles

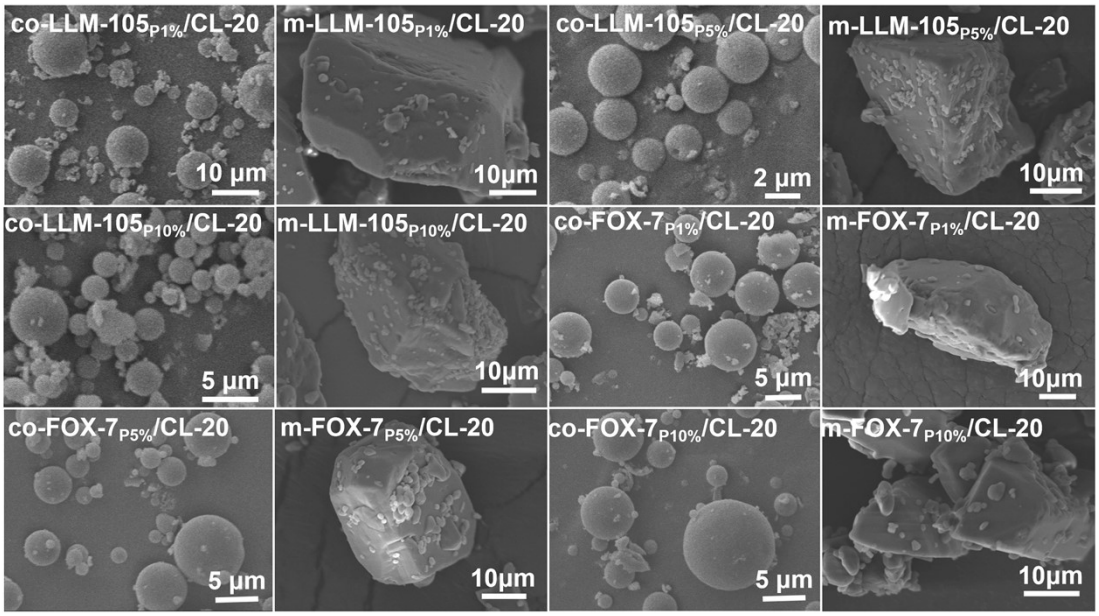

Figure S6 The SEM images of the raw CL-20, co-particles and mixtures

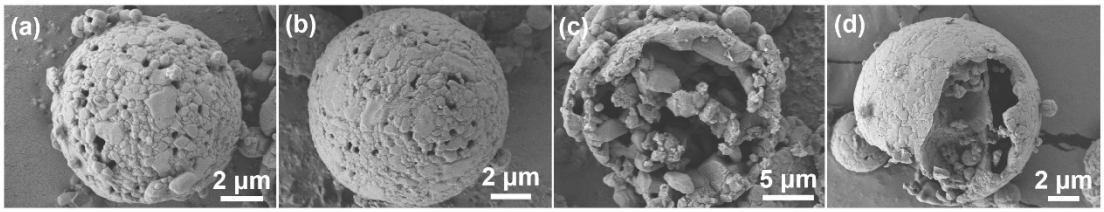

Figure S7 The SEM images of co-LLM-$105_{10\%}$/CL-20 (a), co-FOX-$7_{10\%}$/CL-20, co-LLM-$105_{P10\%}$/CL-20 and co-FOX-$7_{P10\%}$/CL-20 co-particles

S4 The structure of co-particles

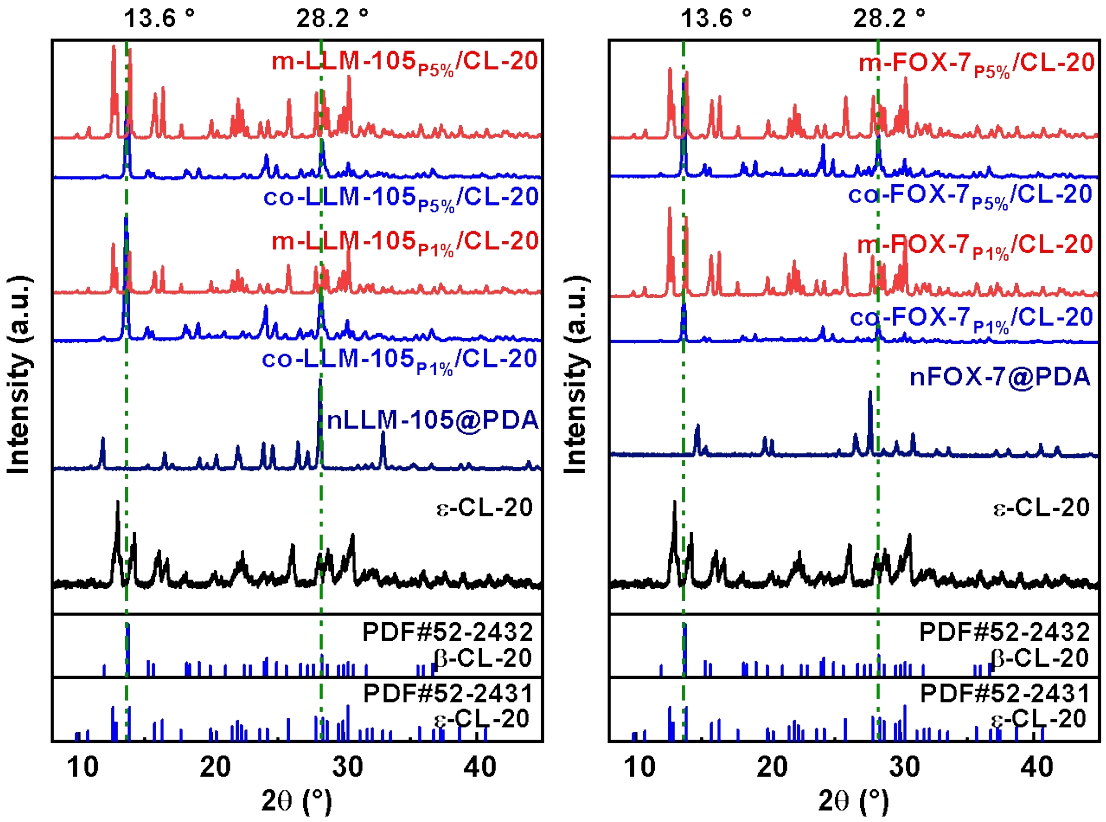

Figure S8 XRD pattern of raw CL-20, co-LLM-105$_P$/CL-20 and co-FOX-7$_P$/CL-20 co-particles

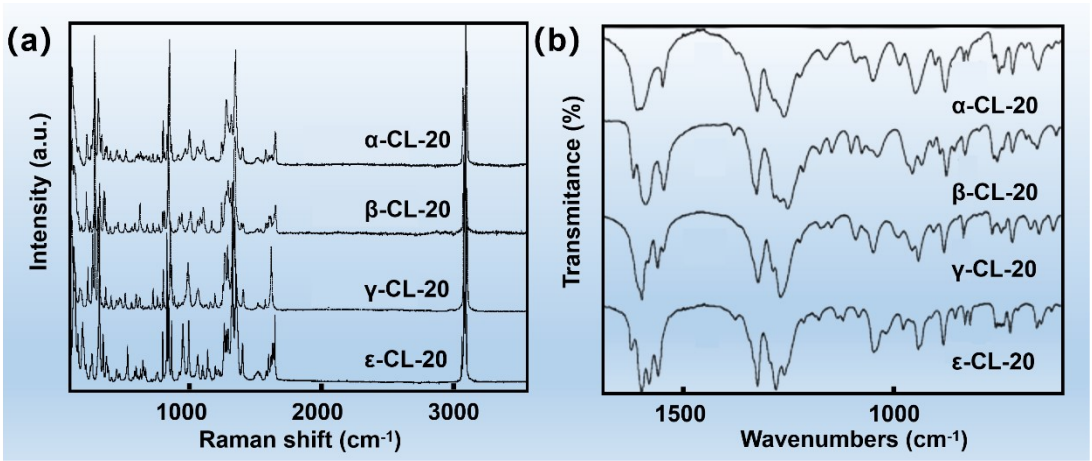

Figure S9 Raman spectrum (a) and IR spectra (b) of CL-20

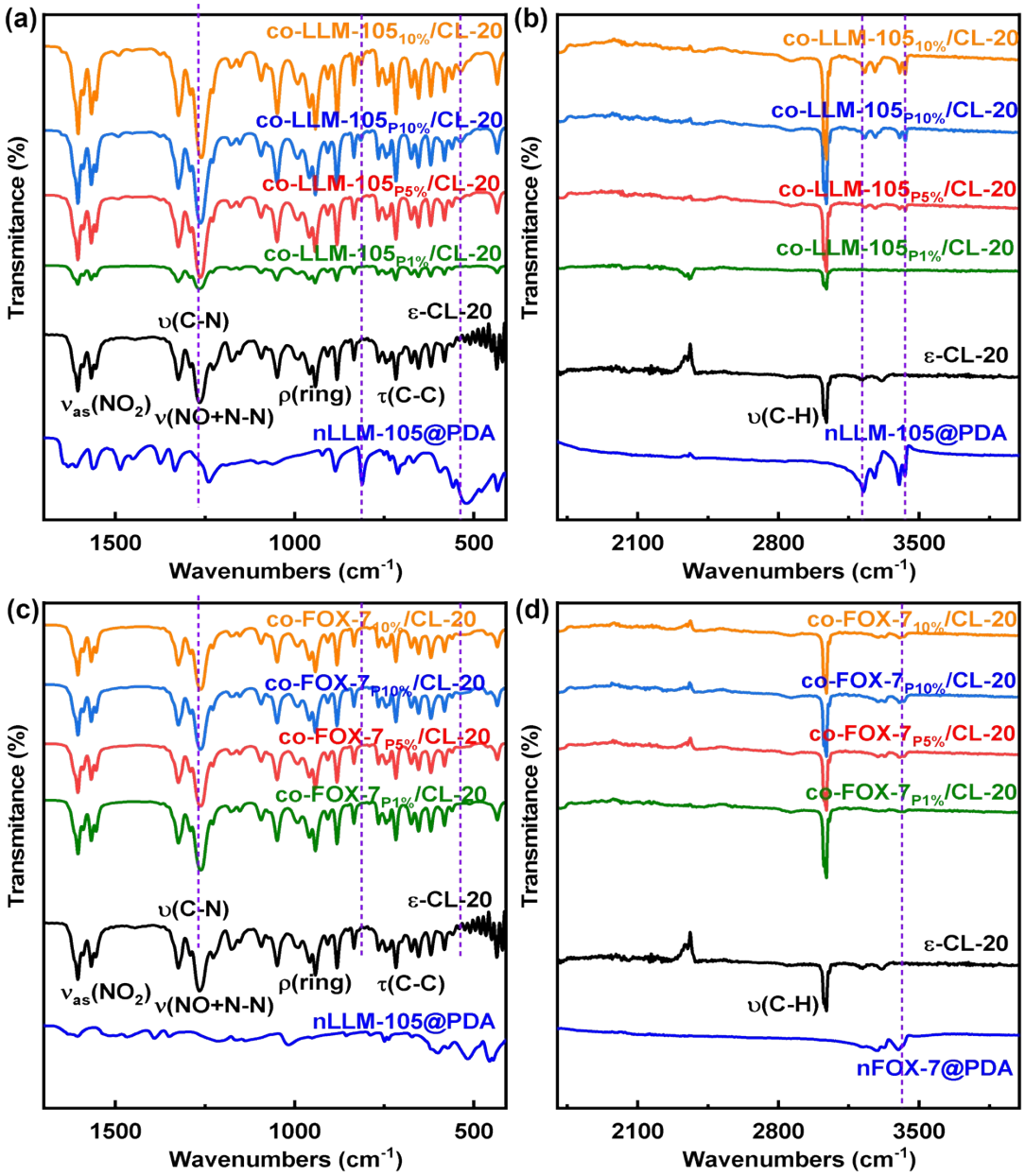

Figure S10 IR spectra of CL-20, co-LLM-105$_P$/CL-20 (a and b) and co-FOX-7$_P$/CL-20 (c and d) co-particles

IR spectroscopy was a supplementary technique for detecting of changes and possible chemical interactions between nLLM-105@PDA, nFOX-7@PDA, and CL-20. The IR spectra of the four crystal forms of CL-20 depicted in **Figure** S9 are consistent with previously reported results in the literature[1]. **Figure** 5 illustrates the infrared spectra of raw CL-20, nLLM-105@PDA, nFOX-7@PDA, co-LLM-105$_P$/CL-20, and co-FOX-7$_P$/CL-20 co-particles. The four absorption peaks of nLLM-105@PDA in the range of 4000-3000 cm^{-1} correspond to the stretching vibration peaks of -NH. In nLLM-105@PDA crystals, a substantial number of -NH_2 and -NO_2 form intermolecular and intramolecular hydrogen bonds, causing the two -NH_2 to be non-equivalent and producing four small peaks. The banding observed in co-LLM-105$_P$/CL-20 co-particles is like that of the raw

material, but some differences remain. The peak intensity in the range of 4000-3000 cm^{-1} slowly increases with the rise of nLLM-105@PDA content in co-particles.

The characteristic peaks associated with CL-20 and nFOX-7@PDA were observed in specific spectral regions of co-FOX-7_P/CL-20 co-particles, namely the range of 4000-1300 cm^{-1} and the fingerprint region of 1300-400 cm^{-1}. These observations indicate that the fundamental molecular structure of CL-20 and nFOX-7@PDA remained unchanged during the formation of the co-particles. The stretching vibration peak of the amino group (-NH_2) assigned to nFOX-7@PDA at 3403 cm^{-1} shifted to 3417 cm^{-1} upon incorporation into the co-FOX-$7_{P10\%}$/CL-20 co-particle. Moreover, as the content of nFOX-7@PDA increased in the co-particle, the intensity of peaks in the range of 3000-3500 cm^{-1} gradually increased. These findings provide evidence for the formation of N-O···H-type hydrogen bonds between the -NO_2 group of CL-20 and the -NH_2 group of nFOX-7@PDA. Additionally, a weak possibility exists for the formation of a C-H···O-N hydrogen bond between the methylene-CH_2 group of CL-20 and the -NO_2 group of nFOX-7@PDA.

Compared with CL-20, new diffraction peaks appear at 813.3 and 530.3 cm^{-1} for co-LLM-105_P/CL-20 co-particle. Based on this analysis, we infer the presence of hydrogen bonding interactions between CL-20 (-NO_2) and LLM-105 (-NH_2) molecules. The stretching vibration absorption peaks of –NO_2 present in raw material CL-20 are 1568 and 1267 cm^{-1}. In the co-LLM-$105_{P10\%}$/CL-20 co-particle, the characteristic absorption peaks of NO_2 are at 1566 and 1262 cm^{-1}. This observation may be due to the diverse chemical environment where NO_2 resides, indicating the formation of hydrogen bonds in co-LLM-$105_{P10\%}$/CL-20 co-particles.

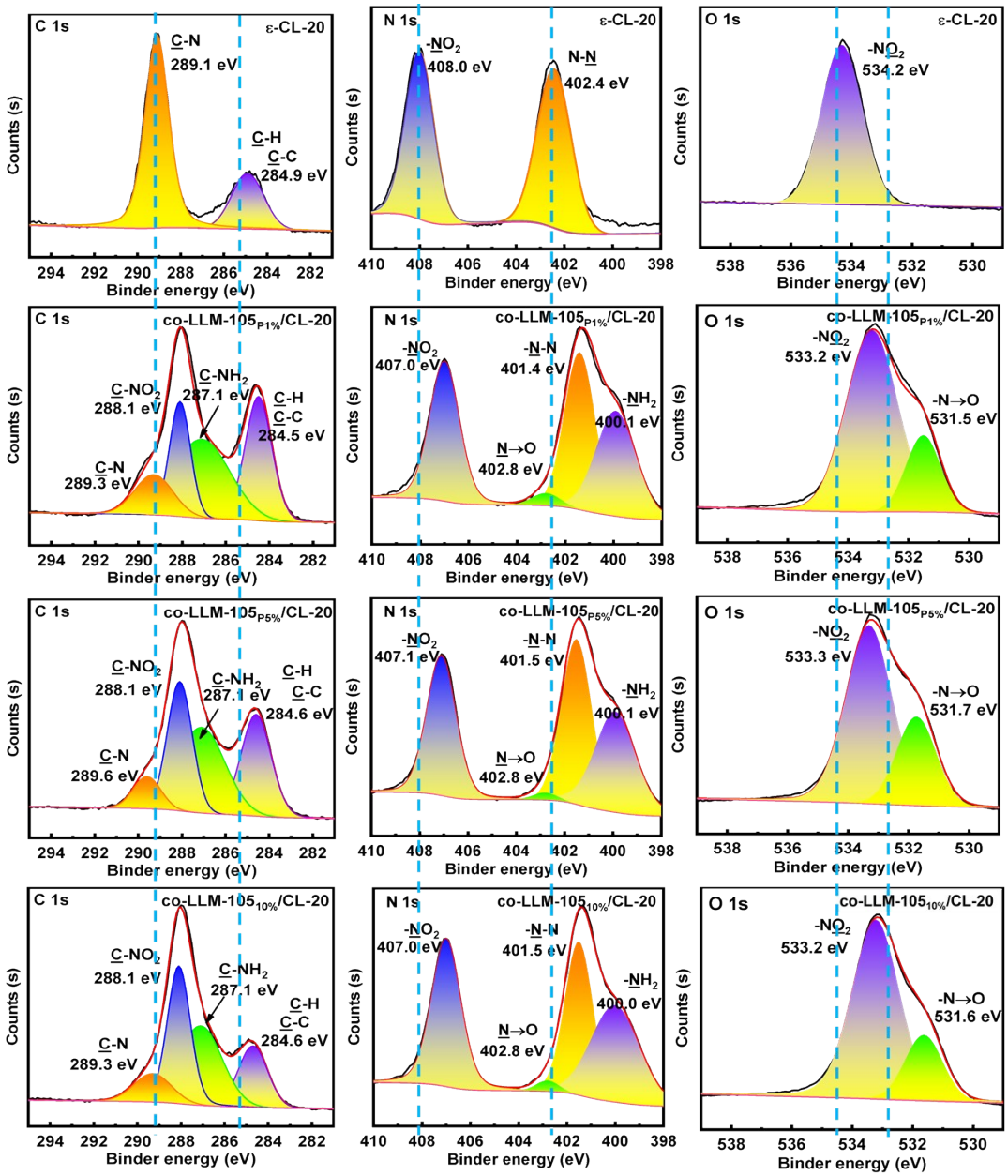

Figure S11 XPS pattern of co-LLM-105$_P$/CL-20 co-particles

Table S1 XPS atomic concentration of functional groups in all atoms of co-LLM-105$_P$/CL-20

Atom	Peak position / eV	Assignment	CL-20 / %	co-LLM-105$_{P1\%}$/CL-20 / %	co-LLM-105$_{P5\%}$/CL-20 / %	co-LLM-105$_{P10\%}$/CL-20 / %	co-LLM-105$_{10\%}$/CL-20 / %
C 1s	284.9	C-C, C -H	19.34	8.90	7.01	7.82	5.37
	287.1	C –NH_2		12.03	9.46	11.14	10.78
	288.1	C –NO_2		6.51	9.66	8.98	10.14
	289.1	C -N	9.62	4.29	2.34	4.72	3.58
N 1s	399.6	C-NH_2		9.10	9.19	10.91	10.56
	402.4	N-N	17.27	11.39	12.75	9.11	11.43
	402.7	N→O		1.27	1.17	1.84	1.20
	408.0	-NO_2	20.61	8.60	9.63	9.77	10.48
O 1s	531.7	-N→O		6.38	7.98	11.70	9.81
	534.2	-NO_2	33.16	31.53	30.83	24.00	26.65

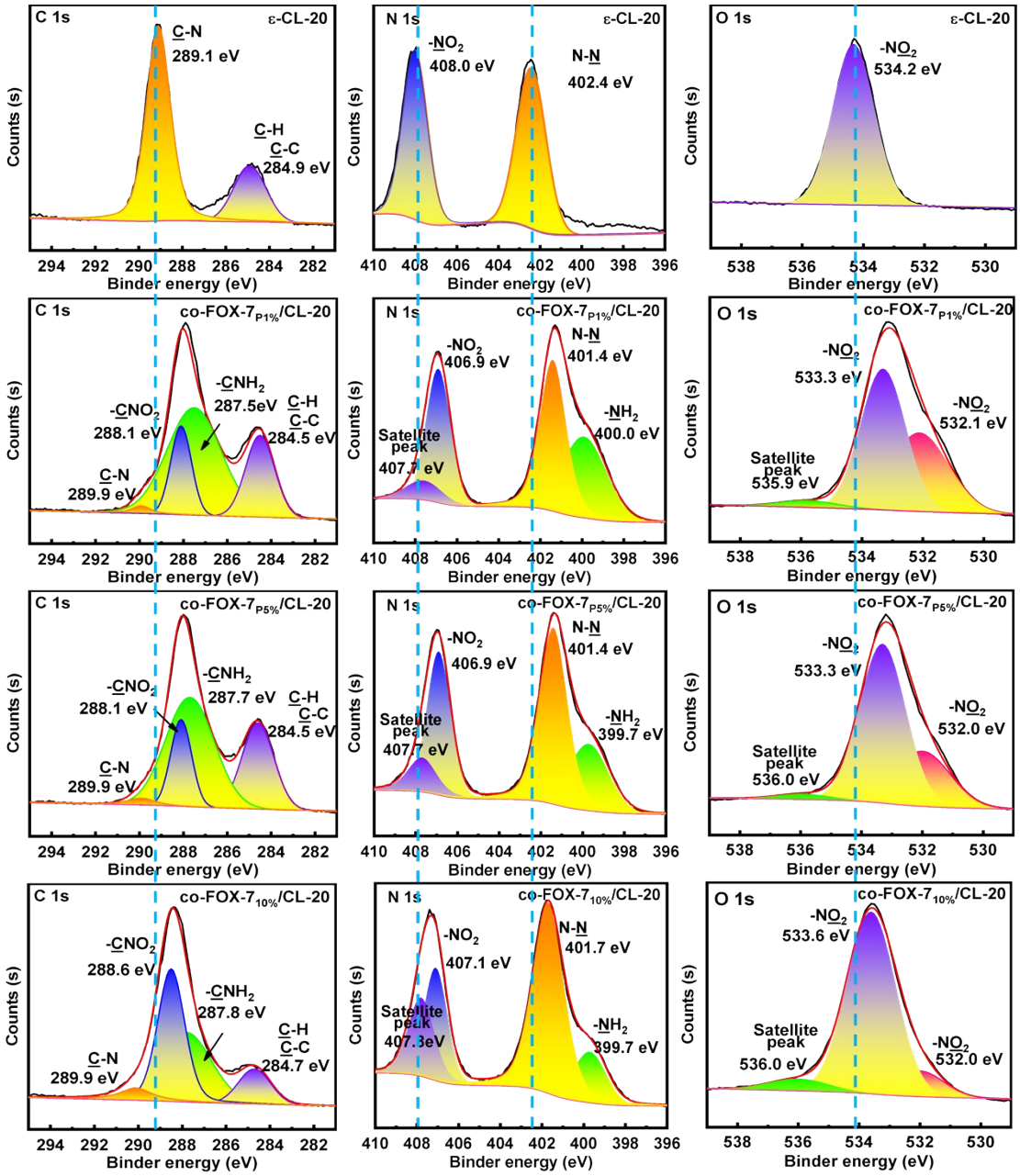

Figure S12 XPS pattern of co-FOX-7$_P$/CL-20 co-particles

Table S2 XPS atomic concentration of functional groups in all atoms of co-FOX-7_P/CL-20

Atom	Peak position / eV	Assignment	CL-20 / %	co-FOX-$7_{P1\%}$/CL-20 / %	co-FOX-$7_{P5\%}$/CL-20 / %	co-FOX-$7_{P10\%}$/CL-20 / %	co-FOX-$7_{10\%}$/CL-20 / %
C 1s	284.5	C-C, C -H	19.34	6.62	7.25	7.50	4.45
	287.6	-CNH_2		15.00	16.39	16.94	10.89
	288.1	-CNO_2		6.59	6.40	6.61	9.53
	289.1	C-N	9.62	3.92	2.41	2.49	4.27
N 1s	402.4, 401.4	N-N	17.27	10.11	10.75	12.47	13.78
	408.0, 406.9	-NO_2	20.61	8.87	9.00	7.46	9.42
	400.0	-NH_2		10.01	7.80	5.36	5.67
	407.7	Satellite peak		4.85	5.91	7.34	8.02
O 1s	531.7	-N→O					
	534.2, 533.3	-NO_2	33.16	14.26	14.88	16.36	18.00
	532.1	-NO_2		12.90	8.76	9.82	7.63
	535.9	Satellite peak		6.87	10.46	7.65	8.36

S5 The thermal stability of co-particles

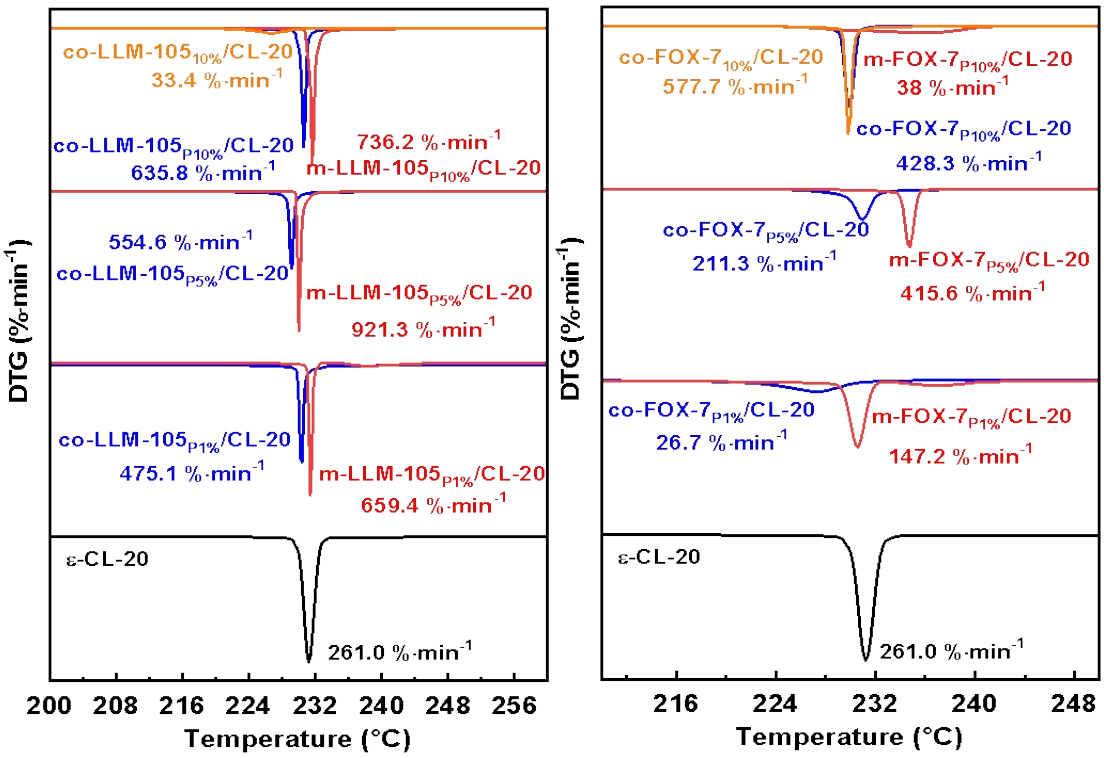

Figure S13 The DTG curves of co-LLM-105$_P$/CL-20 and co-FOX-7$_P$/CL-20 co-particles

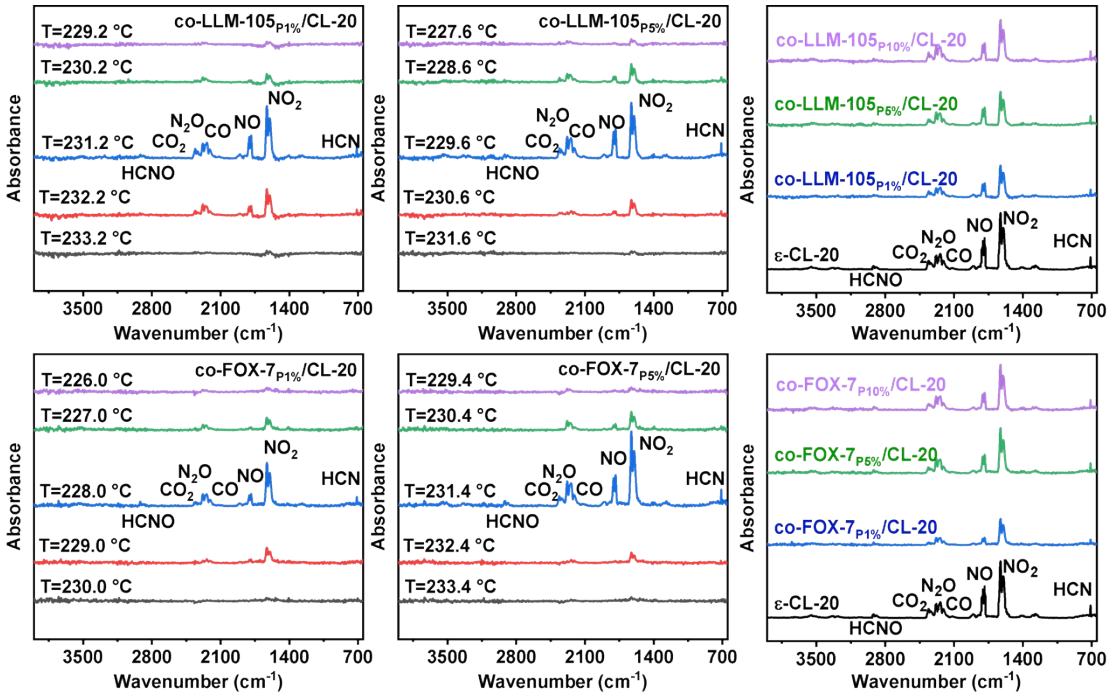

Figure S14 The in-situ FT-IR spectrum of raw CL-20, co-LLM-105$_P$/CL-20 and co-FOX-7$_P$/CL-20 co-particles

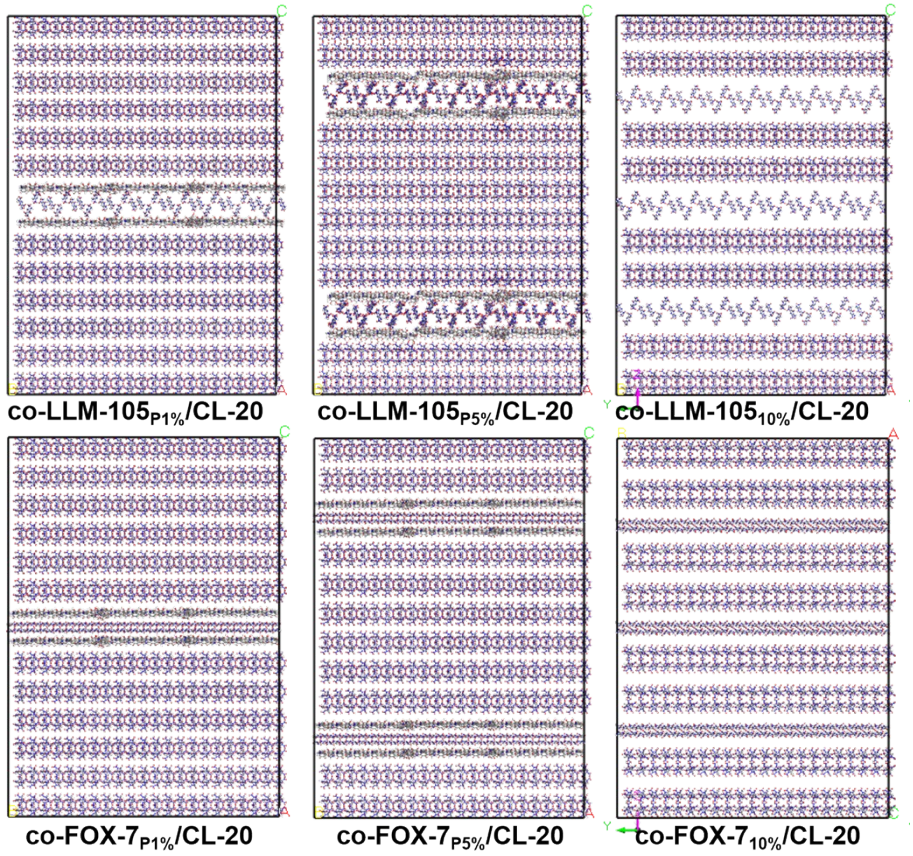

Figure S15 The construction processes of co-LLM-105$_P$/CL-20 and co-FOX-7$_P$/CL-20 co-particles

The cell parameters for β-CL-20 can be accessed from the CCDC crystal library. This compound crystallizes in the orthorhombic system with the space group P21/C. Its initial crystal parameters are (a = 6.540) Å, (b = 11.050) Å, (c = 8.700) Å, with a density of 1.894 g/cm³. The cell parameters for ε-CL-20, also available from the CCDC crystal library, belong to the monoclinic system and have the space group P21/A. These parameters are (a = 13.696) Å, (b = 12.554) Å, (c = 8.833) Å, with a density of 1.894 g/cm³. FOX-7's cell parameters, obtained from the CCDC crystal library, place it in the monoclinic system with space group P21/n, featuring initial crystal parameters of (a = 6.928) Å, (b = 6.620) Å, (c = 11.323) Å, and a density of 1.894 g/cm³. Lastly, the cell parameters for LLM-105 are listed in the CCDC crystal library as belonging to the monoclinic system with the space group C2/C, with initial parameters (a = 14.864) Å, (b = 7.336) Å, (c = 7.509) Å, and maintaining a density of 1.894 g/cm³.

Sandwich models of co-LLM-105P/CL-20 and co-FOX-7p/CL-20 coparticles, containing varying nTATB@PDA concentrations (1%, 5%, 10%), were respectively constructed as shown in Fig. S14. The obtained models were relaxed using the Forcite Geometry Optimization module within the Materials Studio software. The relaxation process was conducted at 300 K for a simulation duration of 5 ps, continuing until the system's energy minimized and stabilized. Subsequently, the LAMMPS module in MAPS software facilitated the high-temperature decomposition simulation of the relaxed sandwich models. The simulations were performed at a temperature of 3000 K, utilizing the NVT ensemble, with a timestep of 0.1 fs. Atomic data from the system was recorded every 1000 steps over a reaction period of 5 ps. The Berendsen temperature control method was employed, setting the damping constant to 20 fs. Visualization was

accomplished using Ovito software. The chemical interactions among the coparticle components at 3000 K were analyzed by examining the decomposition and intermediate product data.

Table S3 Main reactions of the formation of partial gas-phase products of CL-20 decomposition

Gas-phase products	Maximum mole fraction of the gases per mole of CL-20								
	ε-CL-20	LLM-105$_{P1\%}$/CL-20	LLM-105$_{P5\%}$/CL-20	LLM-105$_{P10\%}$/CL-20	LLM-105$_{10\%}$/CL-20	FOX-7$_{P1\%}$/CL-20	FOX-7$_{P5\%}$/CL-20	FOX-7$_{P10\%}$/CL-20	FOX-7$_{10\%}$/CL-20
N_2O	0.10	0.11	0.12	0.13	0.16	0.10	0.10	0.13	0.14
NO	0.56	0.74	0.86	0.96	1.00	0.69	0.73	0.87	1.05
N_2O_4	0.16	0.12	0.10	0.07	0.07	0.12	0.09	0.07	0.06
N_2O_3	0.08	0.06	0.06	0.05	0.05	0.06	0.06	0.05	0.05
NO_3	0.37	0.36	0.31	0.31	0.28	0.38	0.35	0.28	0.29
N_2O_2	0.26	0.27	0.25	0.25	0.18	0.25	0.19	0.22	0.21
NO_2	3.19	3.75	3.77	3.91	4.23	3.47	3.77	3.68	4.31
O_2	0.13	0.10	0.11	0.11	0.12	0.13	0.07	0.08	0.13
N_2	1.19	0.88	0.82	0.82	0.68	0.92	0.83	0.81	0.71
HNO	0.28	0.32	0.38	0.45	0.32	0.31	0.33	0.43	0.35
HNO_3	0.25	0.22	0.19	0.19	0.15	0.24	0.21	0.17	0.17
HNO_2	0.43	0.49	0.52	0.54	0.57	0.47	0.47	0.54	0.55
OH	0.08	0.09	0.12	0.12	0.11	0.08	0.09	0.10	0.10
O_2H_2	0.05	0.04	0.05	0.04	0.03	0.04	0.03	0.04	0.04
OH_2	0.47	0.57	0.70	0.95	0.59	0.59	0.69	0.99	0.62
NCO	0.06	0.11	0.13	0.12	0.16	0.11	0.10	0.11	0.16
N_2CO_2	0.04	0.05	0.05	0.04	0.05	0.05	0.03	0.04	0.05
CO_2	0.10	0.09	0.08	0.06	0.04	0.07	0.13	0.05	0.05
CHON	0.05	0.08	0.09	0.11	0.10	0.08	0.11	0.11	0.12
CHO_4N_4	0.04	0.06	0.06	0.06	0.05	0.05	0.04	0.06	0.07
CHO_2N_3	0.03	0.06	0.07	0.07	0.09	0.04	0.05	0.05	0.10
CHN_2	0.03	0.07	0.08	0.10	0.13	0.05	0.07	0.08	0.12
CHN	0.10	0.21	0.28	0.34	0.40	0.18	0.30	0.29	0.39
$C_6H_6O_8N_{10}$	0.33	0.32	0.35	0.34	0.33	0.34	0.32	0.34	0.34
$C_6H_6O_6N_9$	0.25	0.27	0.26	0.26	0.28	0.25	0.32	0.26	0.26
$C_6H_6O_4N_8$	0.15	0.19	0.19	0.15	0.18	0.16	0.19	0.17	0.17

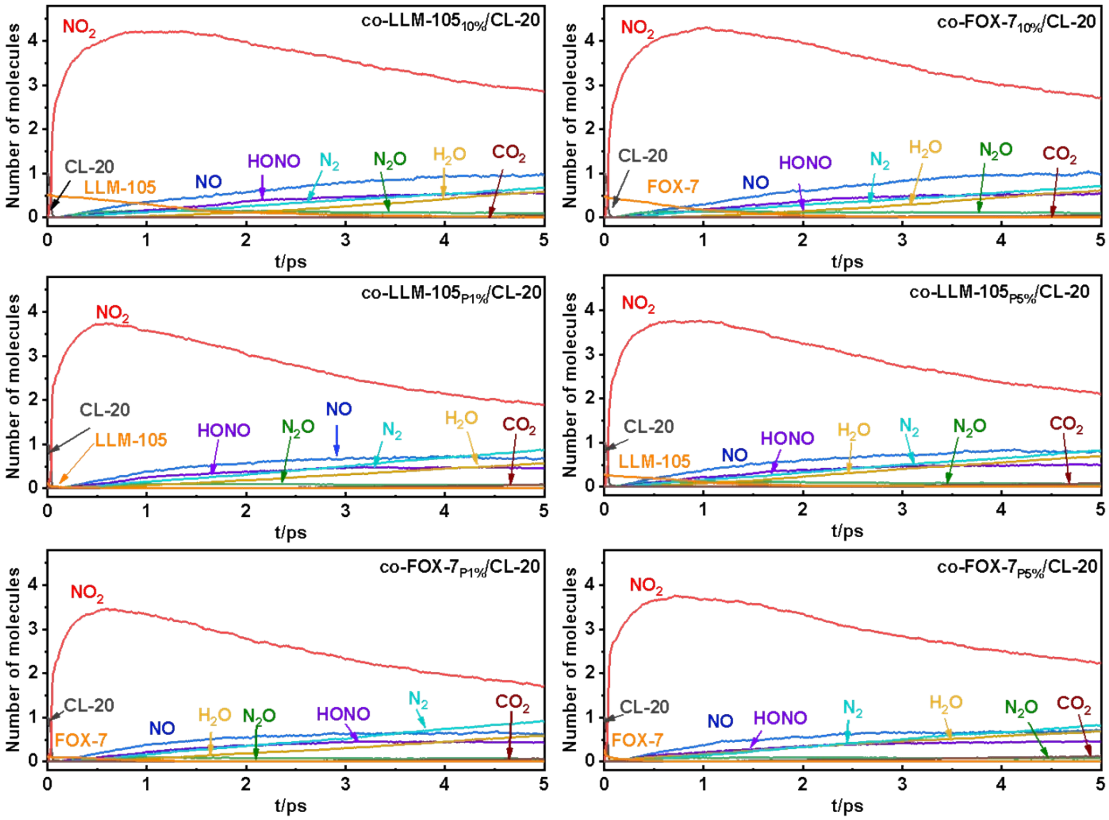

Figure S16 The major initial decomposition fragments of co-LLM-105$_P$/CL-20 and co-FOX-7$_P$/CL-20 co-particles

S6 The kinetic parameter co-particle by Kissinger method

Table S4 Formulations of co-particle and mixture by Kissinger method

Sample	T_P/℃			E_a	Log A	r
	2.5 K·min^{-1}	5 K·min^{-1}	7.5 K·min^{-1}			
ε-CL-20	227.3	231.8	236.9	239.3	18.7	0.9952
co-LLM-105$_{P1\%}$/CL-20	224.5	231.2	233.6	234.0	18.3	0.9945
co-LLM-105$_{P5\%}$/CL-20	222.5	229.6	235.2	175.7	12.2	0.9977
co-LLM-105$_{P10\%}$/CL-20	225.5	230.8	236.0	217.5	16.5	0.9942
co-FOX-7$_{P1\%}$/CL-20	224.0	230.8	234.2	214.3	16.2	0.9992
co-FOX-7$_{P5\%}$/CL-20	225.8	231.4	237.8	223.1	17.1	0.9969
co-FOX-7$_{P10\%}$/CL-20	224.1	230.4	236.0	189.9	13.7	0.9955

S7 The heat of explosion and density

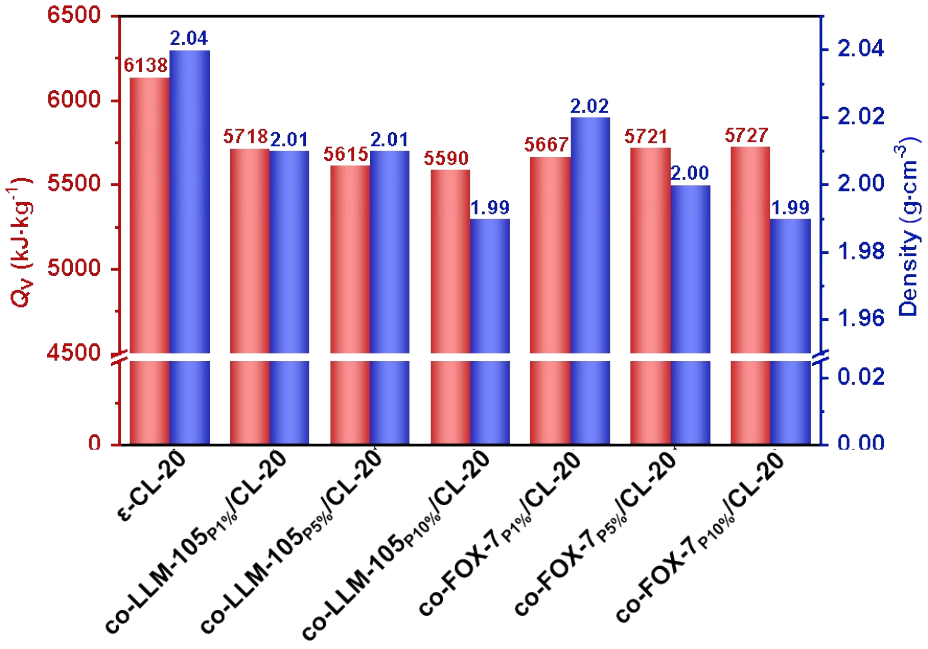

Figure S17 The heat of explosion and density of the raw ε-CL-20, co-LLM-105$_P$/CL-20 and co-FOX-7$_P$/CL-20 co-particles

The heat of explosion (Q_v) serves as a vital parameter commonly utilized to characterize the energy density of energetic materials. Hence, the Q_v of co-LLM-105$_P$/CL-20 and co-FOX-7$_P$/CL-20 co-particles under a 3 MPa pressure was determined using an oxygen bomb calorimeter in an Ar atmosphere (**Figure** 9). The Q_v values for HMX and CL-20 were measured at 5223 and 6138 J·g^{-1}, respectively. The Q_v of co-LLM-105$_{P1\%}$/CL-20 co-particles reached 5718 J·g^{-1}, lower than CL-20 but higher than HMX. With an increase in nLLM-105@PDA content, the Q_v gradually decreased, though remaining higher than that of HMX. Conversely, for co-FOX-7$_P$/CL-20 co-particles, the Q_v increased gradually with higher nFOX-7@PDA content, reaching 5727 J·g^{-1} for co-FOX-7$_{P10\%}$/CL-20. This indicates an enhanced interaction between CL-20 and nFOX-7@PDA, leading to shorter bond lengths. Overall, β-CL-20 exhibits increased mechanical sensitivity and a lower density of 1.98 g·cm^{-3} compared to ε-CL-20. However, the co-particle densities of co-LLM-105$_P$/CL-20 and co-FOX-7$_P$/CL-20 surpass 1.98 g·cm^{-3}, with co-LLM-105$_{P1\%}$/CL-20 and co-FOX-7$_{P1\%}$/CL-20 densities at 2.01 and 2.02 g·cm^{-3}, respectively.

S8 Detonation velocity calculations of co-particles

The original data record of detonation velocity calculation

co-LLM-105$_{P1\%}$/CL-20:

RESULTS OF CALCULATION:

Job title : Test calculation

Comment :

Reactant information:

---

1. XRX, 100 %

C(6.000) H(7.140) N(11.770) O(12.650)

Molecular weight = 446.52

Density of explosive = 2.01 g/cm3

Oxygen balance = -10.46252 %

Enthalpy of formation = 686.56 kJ/kg

Internal energy of formation = 774.16 kJ/kg

Detonation parameters (at the C-J point) :

Heat of detonation = -6265.014 kJ/kg

Detonation temperature = 4088.886 K

Detonation pressure = 43.44427 GPa

Detonation velocity = 9645.187 m/s

Particle velocity = 2240.917 m/s

Sound velocity = 7404.27 m/s

Density of products = 2.61833 g/cm3

Volume of products = 0.3819228 cm3/g

Exponent 'Gamma' = 3.304125

Moles of gaseous products = 13.19936 mol/mol explosive

Moles of condensed products = 1.394929E-10 mol/mol explosive

Volume of gas at STP = 722.9341 dm3/kg

Mean molecular mass of gas. prod. = 33.82819 g/mol

Mean molecular mass of cond.prod. = 12.011 g/mol

Mean molecular mass of all prod. = 33.82819 g/mol

Entropy of products = 6.603571 kJ/kg K

Internal energy of products = 8775.874 kJ/kg, i.e. 17.63951 kJ/cm3

Compression energy = 2510.861 kJ/kg, i.e. 5.04683 kJ/cm3

Total heat energy = -6265.014 kJ/kg, i.e. -12.59268 kJ/cm3

Composition of detonation products:

Products	mol/mol	mol/kg	Mol %
N2 =	5.878397E00	1.316495E01	44.5355
CO2 =	3.103204E00	6.949774E00	23.5103
CH2O2 =	2.242408E00	5.021980E00	16.9888

H2O =	1.308015E00	2.929364E00	9.9097
CO =	6.505391E-01	1.456914E00	4.9286
NH3 =	9.313159E-03	2.085727E-02	0.0706
HCN =	3.644860E-03	8.162839E-03	0.0276
H2 =	3.501881E-03	7.842630E-03	0.0265
CNO =	9.976201E-05	2.234218E-04	0.0008
CH4 =	7.270391E-05	1.628239E-04	0.0006
NO2 =	5.356899E-05	1.199703E-04	0.0004
N2H4 =	2.816991E-05	6.308787E-05	0.0002
H =	2.591155E-05	5.803017E-05	0.0002
NH2 =	2.475405E-05	5.543789E-05	0.0002
CH3OH =	1.022611E-05	2.290186E-05	0.0001
N =	8.652160E-06	1.937693E-05	0.0001
C2H4 =	8.518639E-06	1.907790E-05	0.0001
N2O =	2.626152E-06	5.881393E-06	0.0000
C2H6 =	1.338248E-06	2.997071E-06	0.0000
CHNO =	1.156797E-06	2.590703E-06	0.0000
CH2O =	8.128212E-07	1.820352E-06	0.0000
C(d) =	9.428975E-11	2.111664E-10	0.0000
C(gr) =	4.520318E-11	1.012347E-10	0.0000

Running parameters:

- Equation of state: BKW EOS
- 'BKWN' set of constants
- Covolumes set 1
  (Alpha=0.5, Beta=0.38, Kappa=9.32, Theta=4120)
- Activity: Model 1: Condensed products form pure phase (Default)
- DataBase: D:\EXPLO5_V6.02\explo5 数据库\fengchenhe.xls

********** NEW RUN **********

co-LLM-105$_{P5\%}$/CL-20:

RESULTS OF CALCULATION:

Job title : Test calculation

Comment :

Reactant information:

---

1. XRX-2, 100 %

C(6.000) H(6.530) N(11.490) O(12.060)

Molecular weight = 432.54

Density of explosive = 2.01 g/cm3

Oxygen balance = -11.85475 %

Enthalpy of formation = 684.47 kJ/kg

Internal energy of formation = 770.65 kJ/kg

Detonation parameters (at the C-J point) :

Heat of detonation = -6095.393 kJ/kg
Detonation temperature = 4023.717 K
Detonation pressure = 42.9724 GPa
Detonation velocity = 9587.152 m/s
Particle velocity = 2229.995 m/s
Sound velocity = 7357.157 m/s
Density of products = 2.619242 g/cm3
Volume of products = 0.3817898 cm3/g
Exponent 'Gamma' = 3.299181
Moles of gaseous products = 12.68014 mol/mol explosive
Moles of condensed products = 0.02591983 mol/mol explosive
Volume of gas at STP = 716.9373 dm3/kg
Mean molecular mass of gas. prod. = 34.08658 g/mol
Mean molecular mass of cond.prod. = 12.011 g/mol
Mean molecular mass of all prod. = 34.04155 g/mol
Entropy of products = 6.539052 kJ/kg K
Internal energy of products = 8581.838 kJ/kg, i.e. 17.24949 kJ/cm3
Compression energy = 2486.446 kJ/kg, i.e. 4.997756 kJ/cm3
Total heat energy = -6095.393 kJ/kg, i.e. -12.25174 kJ/cm3

Composition of detonation products:

Products	mol/mol	mol/kg	Mol %
N2 =	5.736127E00	1.326143E01	45.1448
CO2 =	2.851552E00	6.592542E00	22.4425
CH2O2 =	2.285773E00	5.284510E00	17.9896
H2O =	9.558632E-01	2.209873E00	7.5229
CO =	8.293118E-01	1.917297E00	6.5269
C(d) =	2.591983E-02	5.992440E-02	0.2040
NH3 =	1.047630E-02	2.422031E-02	0.0825
HCN =	7.035966E-03	1.626655E-02	0.0554
H2 =	3.539115E-03	8.182128E-03	0.0279
CH4 =	1.774214E-04	4.101830E-04	0.0014
CNO =	1.135312E-04	2.624743E-04	0.0009
C2H4 =	4.068179E-05	9.405278E-05	0.0003
N2H4 =	3.197376E-05	7.392056E-05	0.0003
NH2 =	2.343009E-05	5.416834E-05	0.0002
H =	2.211799E-05	5.113488E-05	0.0002
NO2 =	1.980024E-05	4.577645E-05	0.0002
CH3OH =	1.644902E-05	3.802871E-05	0.0001
C2H6 =	7.570642E-06	1.750267E-05	0.0001
N =	6.494207E-06	1.501404E-05	0.0001
CHNO =	1.518368E-06	3.510335E-06	0.0000
N2O =	1.503865E-06	3.476807E-06	0.0000

CH2O = 1.111262E-06 2.569141E-06 0.0000

C(gr) = 1.759859E-10 4.068642E-10 0.0000

Running parameters:

- Equation of state: BKW EOS
- 'BKWN' set of constants
- Covolumes set 1

  (Alpha=0.5, Beta=0.38, Kappa=9.32, Theta=4120)
- Activity: Model 1: Condensed products form pure phase (Default)
- DataBase: D:\EXPLO5_V6.02\explo5 数据库\fengchenhe.xls

********** NEW RUN **********

co-LLM-105$_{P10\%}$/CL-20:

RESULTS OF CALCULATION:

Job title : Test calculation

Comment :

Reactant information:

---

1. XRD-3, 100 %

C(6.000) H(7.030) N(11.330) O(11.460)

Molecular weight = 421.21

Density of explosive = 1.99 g/cm3

Oxygen balance = -15.40245 %

Enthalpy of formation = 683.97 kJ/kg

Internal energy of formation = 771.71 kJ/kg

Detonation parameters (at the C-J point) :

Heat of detonation = -5964.918 kJ/kg

Detonation temperature = 3931.21 K

Detonation pressure = 41.46445 GPa

Detonation velocity = 9463.573 m/s

Particle velocity = 2201.748 m/s

Sound velocity = 7261.825 m/s

Density of products = 2.593358 g/cm3

Volume of products = 0.3856005 cm3/g

Exponent 'Gamma' = 3.298209

Moles of gaseous products = 12.37679 mol/mol explosive

Moles of condensed products = 0.4654796 mol/mol explosive

Volume of gas at STP = 718.6206 dm3/kg

Mean molecular mass of gas. prod. = 33.57948 g/mol

Mean molecular mass of cond.prod. = 12.011 g/mol

Mean molecular mass of all prod. = 32.79771 g/mol

Entropy of products = 6.573704 kJ/kg K

Internal energy of products = 8388.771 kJ/kg, i.e. 16.69366 kJ/cm3

Compression energy = 2423.854 kJ/kg, i.e. 4.823469 kJ/cm3

Total heat energy = -5964.918 kJ/kg, i.e. -11.87019 kJ/cm3

Composition of detonation products:

Products	mol/mol	mol/kg	Mol %
N2 =	5.653871E00	1.342307E01	44.0255
CO2 =	2.449606E00	5.815703E00	19.0746
CH2O2 =	2.314668E00	5.495344E00	18.0238
H2O =	1.168889E00	2.775104E00	9.1019
CO =	7.624304E-01	1.810115E00	5.9369
C(d) =	4.654796E-01	1.105113E00	3.6246
NH3 =	1.479143E-02	3.511690E-02	0.1152
HCN =	7.256058E-03	1.722689E-02	0.0565
H2 =	4.690945E-03	1.113695E-02	0.0365
CH4 =	2.986647E-04	7.090713E-04	0.0023
CNO =	8.099782E-05	1.923001E-04	0.0006
C2H4 =	6.178270E-05	1.466807E-04	0.0005
N2H4 =	4.226139E-05	1.003344E-04	0.0003
NH2 =	2.589422E-05	6.147646E-05	0.0002
CH3OH =	2.330592E-05	5.533149E-05	0.0002
H =	2.267958E-05	5.384446E-05	0.0002
C2H6 =	1.517684E-05	3.603192E-05	0.0001
NO2 =	1.202113E-05	2.853983E-05	0.0001
N =	4.787115E-06	1.136527E-05	0.0000
CHNO =	1.456141E-06	3.457080E-06	0.0000
CH2O =	1.250869E-06	2.969736E-06	0.0000
N2O =	1.082443E-06	2.569869E-06	0.0000
C(gr) =	1.805606E-10	4.286758E-10	0.0000

Running parameters:

- Equation of state: BKW EOS
- 'BKWN' set of constants
- Covolumes set 1
  (Alpha=0.5, Beta=0.38, Kappa=9.32, Theta=4120)
- Activity: Model 1: Condensed products form pure phase (Default)
- DataBase: D:\EXPLO5_V6.02\explo5 数据库\fengchenhe.xls

********** NEW RUN **********

co-FOX-7$_{P1\%}$/CL-20:

RESULTS OF CALCULATION:

Job title : Test calculation

Comment :

Reactant information:

---

1. XRX-4, 100 %

C(6.000) H(7.170) N(11.800) O(11.750)

Molecular weight = 432.57

Density of explosive = 2.02 g/cm3

Oxygen balance = -14.1841 %

Enthalpy of formation = 734.17 kJ/kg

Internal energy of formation = 822.19 kJ/kg

Detonation parameters (at the C-J point) :

Heat of detonation = -6023.753 kJ/kg

Detonation temperature = 3931.743 K

Detonation pressure = 43.34855 GPa

Detonation velocity = 9621.68 m/s

Particle velocity = 2230.346 m/s

Sound velocity = 7391.334 m/s

Density of products = 2.629538 g/cm3

Volume of products = 0.3802949 cm3/g

Exponent 'Gamma' = 3.313985

Moles of gaseous products = 12.69299 mol/mol explosive

Moles of condensed products = 0.3328318 mol/mol explosive

Volume of gas at STP = 717.6175 dm3/kg

Mean molecular mass of gas. prod. = 33.76379 g/mol

Mean molecular mass of cond.prod. = 12.011 g/mol

Mean molecular mass of all prod. = 33.20797 g/mol

Entropy of products = 6.541676 kJ/kg K

Internal energy of products = 8510.98 kJ/kg, i.e. 17.19218 kJ/cm3

Compression energy = 2487.228 kJ/kg, i.e. 5.024199 kJ/cm3

Total heat energy = -6023.753 kJ/kg, i.e. -12.16798 kJ/cm3

Composition of detonation products:

Products	mol/mol	mol/kg	Mol %
N2 =	5.890473E00	1.361739E01	45.2215
CO2 =	2.530766E00	5.850534E00	19.4288
CH2O2 =	2.439584E00	5.639745E00	18.7288
H2O =	1.118825E00	2.586460E00	8.5893
CO =	6.903517E-01	1.595930E00	5.2999
C(d) =	3.328318E-01	7.694288E-01	2.5552
NH3 =	1.280375E-02	2.959924E-02	0.0983
HCN =	6.055441E-03	1.399875E-02	0.0465
H2 =	3.678740E-03	8.504381E-03	0.0282
CH4 =	2.119651E-04	4.900135E-04	0.0016
CNO =	7.553965E-05	1.746299E-04	0.0006
C2H4 =	4.213348E-05	9.740268E-05	0.0003
N2H4 =	3.796862E-05	8.777452E-05	0.0003

NH2 = 2.084103E-05 4.817955E-05 0.0002

H = 1.771085E-05 4.094332E-05 0.0001

CH3OH = 1.689217E-05 3.905072E-05 0.0001

NO2 = 1.387111E-05 3.206675E-05 0.0001

C2H6 = 9.916893E-06 2.292552E-05 0.0001

N = 4.623505E-06 1.068845E-05 0.0000

N2O = 1.022452E-06 2.363669E-06 0.0000

CHNO = 1.000824E-06 2.313670E-06 0.0000

CH2O = 8.147393E-07 1.883485E-06 0.0000

C(gr) = 1.642749E-10 3.797649E-10 0.0000

Running parameters:

- Equation of state: BKW EOS
- 'BKWN' set of constants
- Covolumes set 1

  (Alpha=0.5, Beta=0.38, Kappa=9.32, Theta=4120)
- Activity: Model 1: Condensed products form pure phase (Default)
- DataBase: D:\EXPLO5_V6.02\explo5 数据库\fengchenhe.xls

********** NEW RUN **********

co-FOX-7$_{P5\%}$/CL-20:

RESULTS OF CALCULATION:

Job title : Test calculation

Comment :

Reactant information:

---

1. XRX-5, 100 %

C(6.000) H(6.190) N(11.570) O(12.220)

Molecular weight = 435.88

Density of explosive = 2.0 g/cm3

Oxygen balance = -10.55271 %

Enthalpy of formation = 690.12 kJ/kg

Internal energy of formation = 775.37 kJ/kg

Detonation parameters (at the C-J point) :

Heat of detonation = -6156.667 kJ/kg

Detonation temperature = 4100.017 K

Detonation pressure = 42.57571 GPa

Detonation velocity = 9562.936 m/s

Particle velocity = 2226.079 m/s

Sound velocity = 7336.856 m/s

Density of products = 2.606821 g/cm3

Volume of products = 0.383609 cm3/g

Exponent 'Gamma' = 3.295865

Moles of gaseous products = 12.81652 mol/mol explosive

Moles of condensed products = 2.576283E-10 mol/mol explosive

Volume of gas at STP = 719.099 dm3/kg

Mean molecular mass of gas. prod. = 34.00861 g/mol

Mean molecular mass of cond.prod. = 12.011 g/mol

Mean molecular mass of all prod. = 34.00861 g/mol

Entropy of products = 6.53652 kJ/kg K

Internal energy of products = 8634.388 kJ/kg, i.e. 17.26878 kJ/cm3

Compression energy = 2477.72 kJ/kg, i.e. 4.955441 kJ/cm3

Total heat energy = -6156.667 kJ/kg, i.e. -12.31334 kJ/cm3

Composition of detonation products:

Products	mol/mol	mol/kg	Mol %
N2 =	5.778044E00	1.325605E01	45.0828
CO2 =	3.149301E00	7.225159E00	24.5722
CH2O2 =	2.049475E00	4.701928E00	15.9909
H2O =	1.026418E00	2.354818E00	8.0086
CO =	7.958044E-01	1.825743E00	6.2092
NH3 =	8.502788E-03	1.950718E-02	0.0663
HCN =	5.149686E-03	1.181446E-02	0.0402
H2 =	3.440503E-03	7.893237E-03	0.0268
CNO =	1.271948E-04	2.918115E-04	0.0010
CH4 =	9.272889E-05	2.127396E-04	0.0007
NO2 =	4.029759E-05	9.245115E-05	0.0003
H =	2.728663E-05	6.260126E-05	0.0002
NH2 =	2.518832E-05	5.778730E-05	0.0002
N2H4 =	2.517083E-05	5.774717E-05	0.0002
C2H4 =	1.526068E-05	3.501120E-05	0.0001
CH3OH =	1.168589E-05	2.680990E-05	0.0001
N =	8.933848E-06	2.049613E-05	0.0001
N2O =	2.520814E-06	5.783278E-06	0.0000
C2H6 =	2.210306E-06	5.070907E-06	0.0000
CHNO =	1.641140E-06	3.765120E-06	0.0000
CH2O =	1.093377E-06	2.508438E-06	0.0000
C(d) =	1.837914E-10	4.216560E-10	0.0000
C(gr) =	7.383687E-11	1.693973E-10	0.0000

Running parameters:

- Equation of state: BKW EOS
- 'BKWN' set of constants
- Covolumes set 1

  (Alpha=0.5, Beta=0.38, Kappa=9.32, Theta=4120)
- Activity: Model 1: Condensed products form pure phase (Default)
- DataBase: D:\EXPLO5_V6.02\explo5 数据库\fengchenhe.xls

********** NEW RUN **********

co-FOX-7$_{P10\%}$/CL-20:

RESULTS OF CALCULATION:

Job title : Test calculation

Comment :

Reactant information:

---

1. XRX-6, 100 %

C(6.000) H(6.500) N(11.780) O(12.300)

Molecular weight = 440.41

Density of explosive = 1.99 g/cm3

Oxygen balance = -10.71652 %

Enthalpy of formation = 628.20 kJ/kg

Internal energy of formation = 714.26 kJ/kg

Detonation parameters (at the C-J point) :

Heat of detonation = -6080.76 kJ/kg

Detonation temperature = 4053.465 K

Detonation pressure = 41.9066 GPa

Detonation velocity = 9513.065 m/s

Particle velocity = 2213.649 m/s

Sound velocity = 7299.416 m/s

Density of products = 2.593495 g/cm3

Volume of products = 0.3855801 cm3/g

Exponent 'Gamma' = 3.297458

Moles of gaseous products = 13.01023 mol/mol explosive

Moles of condensed products = 2.865981E-10 mol/mol explosive

Volume of gas at STP = 722.4525 dm3/kg

Mean molecular mass of gas. prod. = 33.85073 g/mol

Mean molecular mass of cond.prod. = 12.011 g/mol

Mean molecular mass of all prod. = 33.85073 g/mol

Entropy of products = 6.548775 kJ/kg K

Internal energy of products = 8530.887 kJ/kg, i.e. 16.97647 kJ/cm3

Compression energy = 2450.127 kJ/kg, i.e. 4.875753 kJ/cm3

Total heat energy = -6080.76 kJ/kg, i.e. -12.10071 kJ/cm3

Composition of detonation products:

Products	mol/mol	mol/kg	Mol %
N2 =	5.882249E00	1.335618E01	45.2125
CO2 =	3.077268E00	6.987217E00	23.6527
CH2O2 =	2.114083E00	4.800219E00	16.2494
H2O =	1.114194E00	2.529879E00	8.5640
CO =	8.029066E-01	1.823073E00	6.1713

NH3 =	9.811185E-03	2.227719E-02	0.0754
HCN =	5.448735E-03	1.237185E-02	0.0419
H2 =	3.872174E-03	8.792125E-03	0.0298
CH4 =	1.184203E-04	2.688841E-04	0.0009
CNO =	1.141773E-04	2.592500E-04	0.0009
NO2 =	3.221249E-05	7.314140E-05	0.0002
N2H4 =	2.793201E-05	6.342218E-05	0.0002
H =	2.747903E-05	6.239364E-05	0.0002
NH2 =	2.610884E-05	5.928251E-05	0.0002
C2H4 =	1.928104E-05	4.377936E-05	0.0001
CH3OH =	1.371285E-05	3.113628E-05	0.0001
N =	7.848693E-06	1.782117E-05	0.0001
C2H6 =	3.105472E-06	7.051258E-06	0.0000
N2O =	2.192862E-06	4.979094E-06	0.0000
CHNO =	1.664012E-06	3.778290E-06	0.0000
CH2O =	1.175210E-06	2.668421E-06	0.0000
C(d) =	2.080571E-10	4.724126E-10	0.0000
C(gr) =	7.854105E-11	1.783346E-10	0.0000

Running parameters:

- Equation of state: BKW EOS
- 'BKWN' set of constants
- Covolumes set 1
  (Alpha=0.5, Beta=0.38, Kappa=9.32, Theta=4120)
- Activity: Model 1: Condensed products form pure phase (Default)
- DataBase: D:\EXPLO5_V6.02\explo5\fengchenhe.xls

********** NEW RUN **********

References

[1] Ghosh, M.; Venkatesan, V.; Mandave, S.; Banerjee, S.; Sikder, N.; Sikder, A.; Bhattacharya, B. Probing Crystal Growth of ε- and α-CL-20 Polymorphs via Metastable Phase Transition Using Microscopy and Vibrational Spectroscopy. *Cryst. Growth Des.* **2014**, *14*, 5053-5063.