

Supplementary Information

Efficient Construction Core/Double-shelled Structured AP@nano-graphite@F₂₆₀₃ Energetic Microcapsules with Low Sensitivity and Hygroscopicity

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The F_{2603} polymer chain was constructed initially using difluoroethylene and hexafluoropropylene in a molar ratio of 4:1, with a chain length of 5. A spherical AP cluster with a radius of 10 Å was then constructed using the MS software base modeling function and placed at the center of a cubic lattice with a side length of 50 Å. The AP cluster was placed in the center of the body of the cubic lattice. A spherical cluster of C atoms with a radius of 13 Å was constructed using the MS software base modeling function. The core (10 Å) was then manually removed, resulting in a spherical shell-shaped monolayer of carbon atoms. These atoms were subsequently transferred to the spherical AP. Finally, 0.5 g/cm³ of F_{2603} rubber molecules were added to the vacuum space of the cubic lattice using the AC module, ensuring uniform distribution. The initial model is finally obtained.

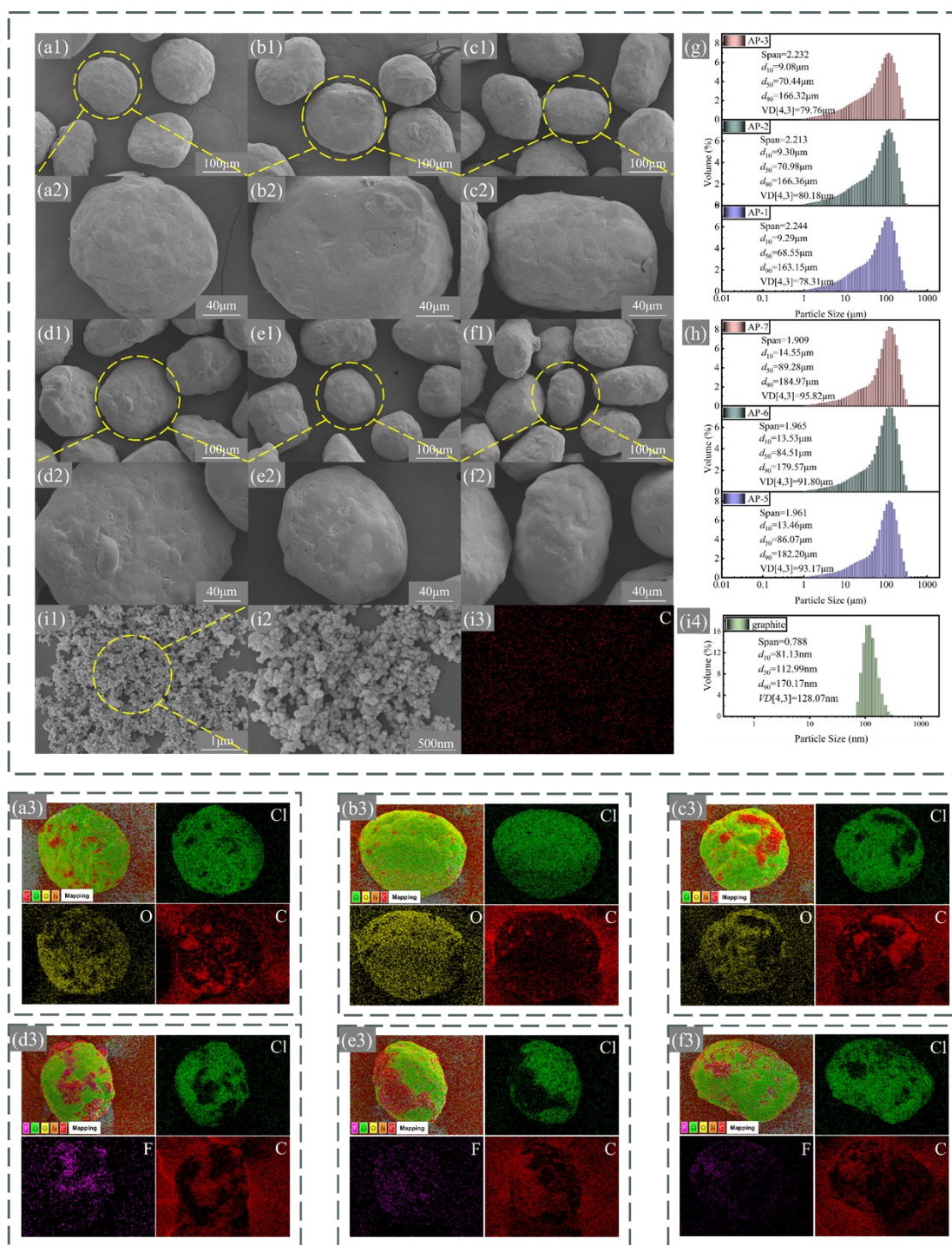


Figure S1. SEM, EDS and particle size analysis of AP-based energetic microcapsules and graphite:

(a1, a2, a3) AP-1; (b1, b2, b3) AP-2; (c1, c2, c3) AP-3; (d1, d2, d3) AP-5; (e1, e2, e3) AP-6; (f1, f2, f3) AP-7; (g, h) particle size; (i1, i2, i3, i4) graphite.

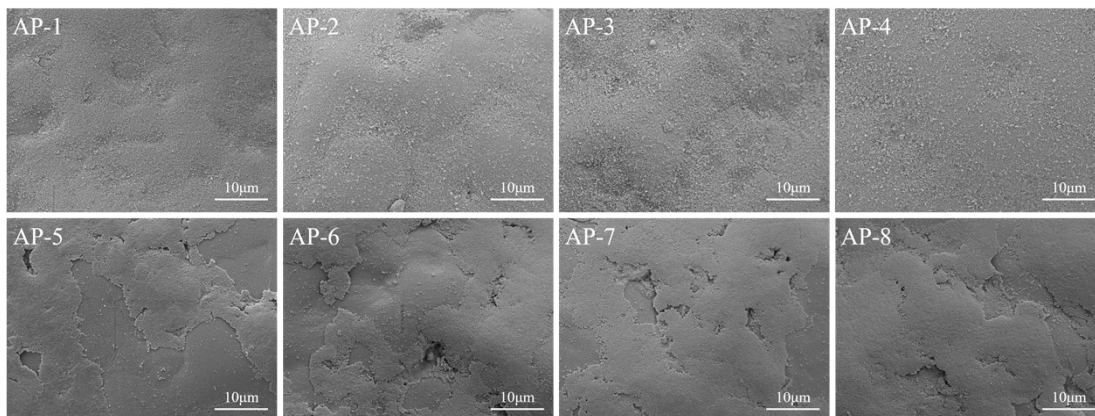


Figure S2. SEM analysis of AP-based energetic microcapsules.

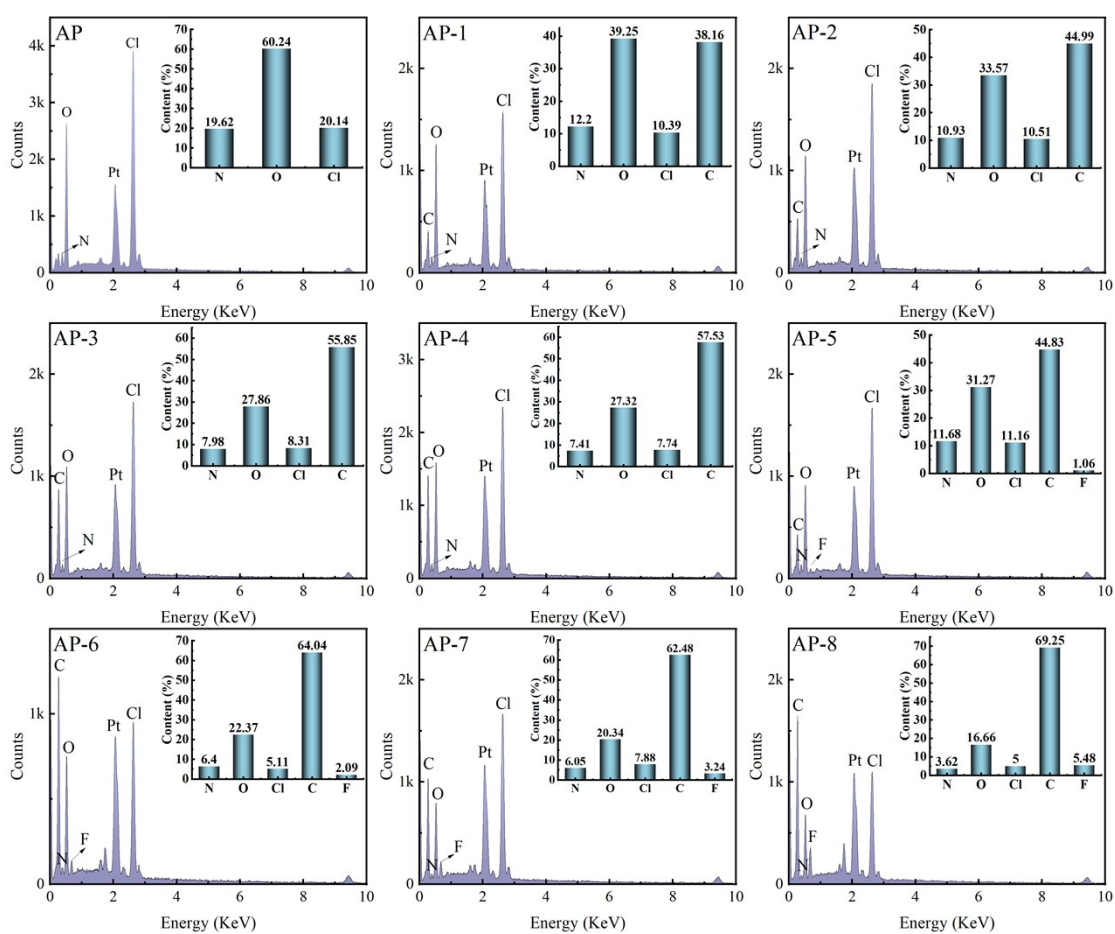


Figure S3. EDS analysis of the different AP-based energetic microcapsules.

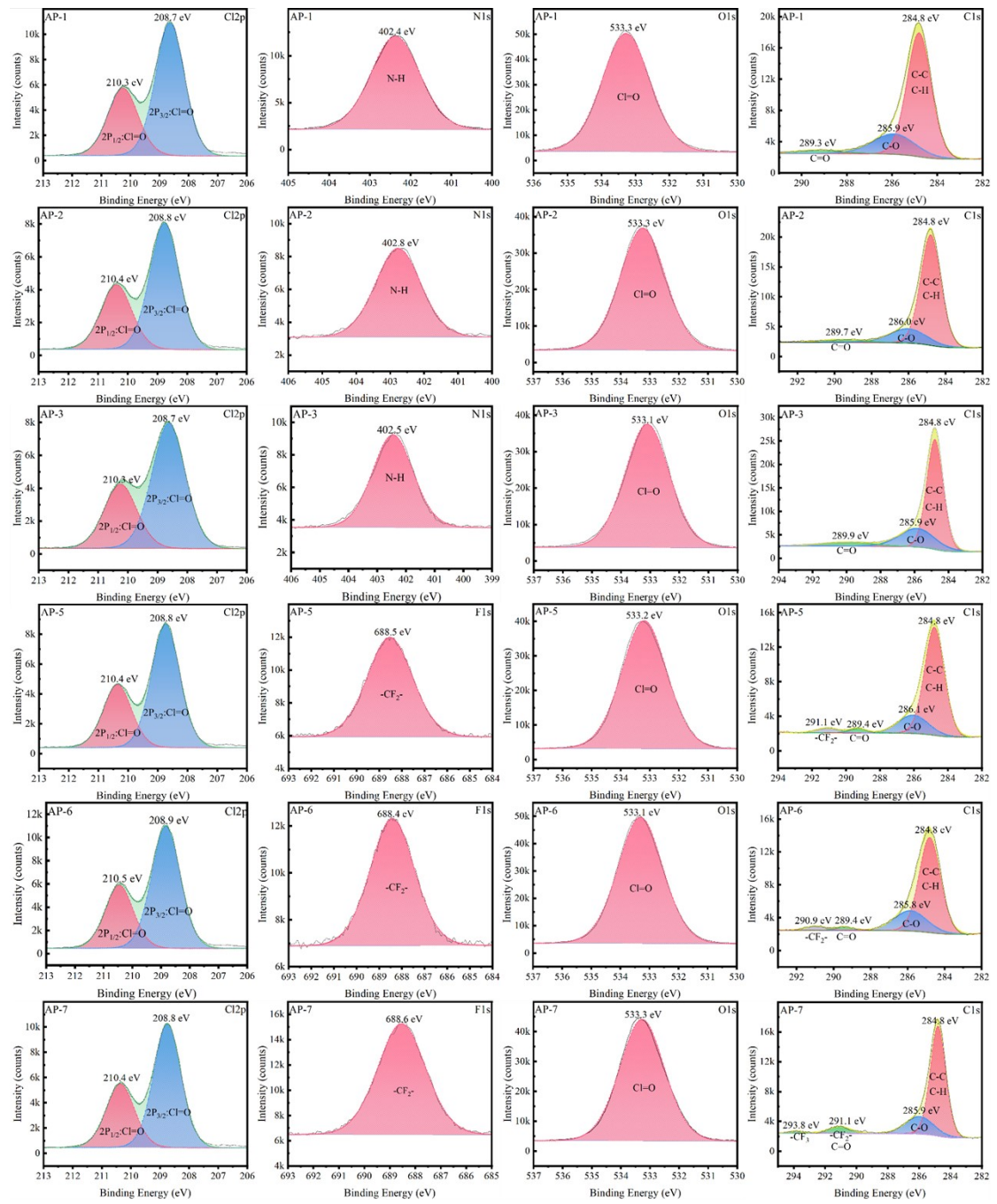


Figure S4. XPS spectra of AP-based energetic microcapsules.

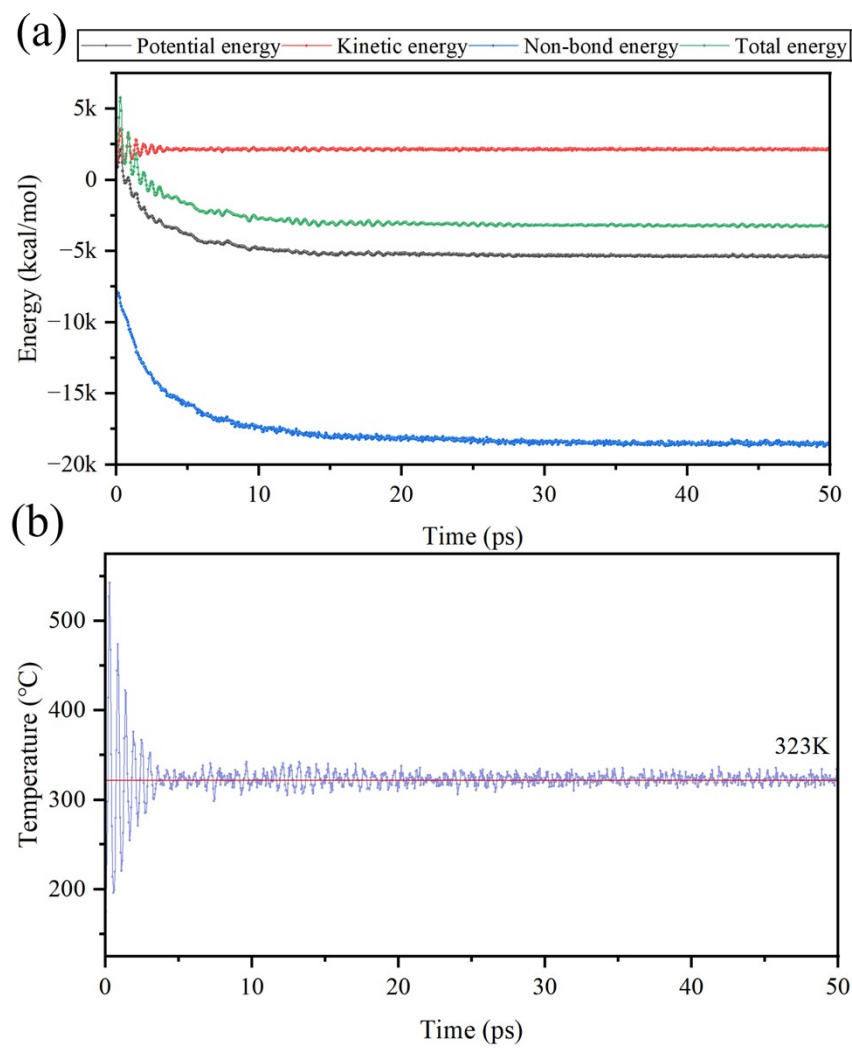


Figure S5. Forcite dynamics energy (a) and forcite dynamics temperature (b) of F_{2603} coated on AP@nano-graphite.

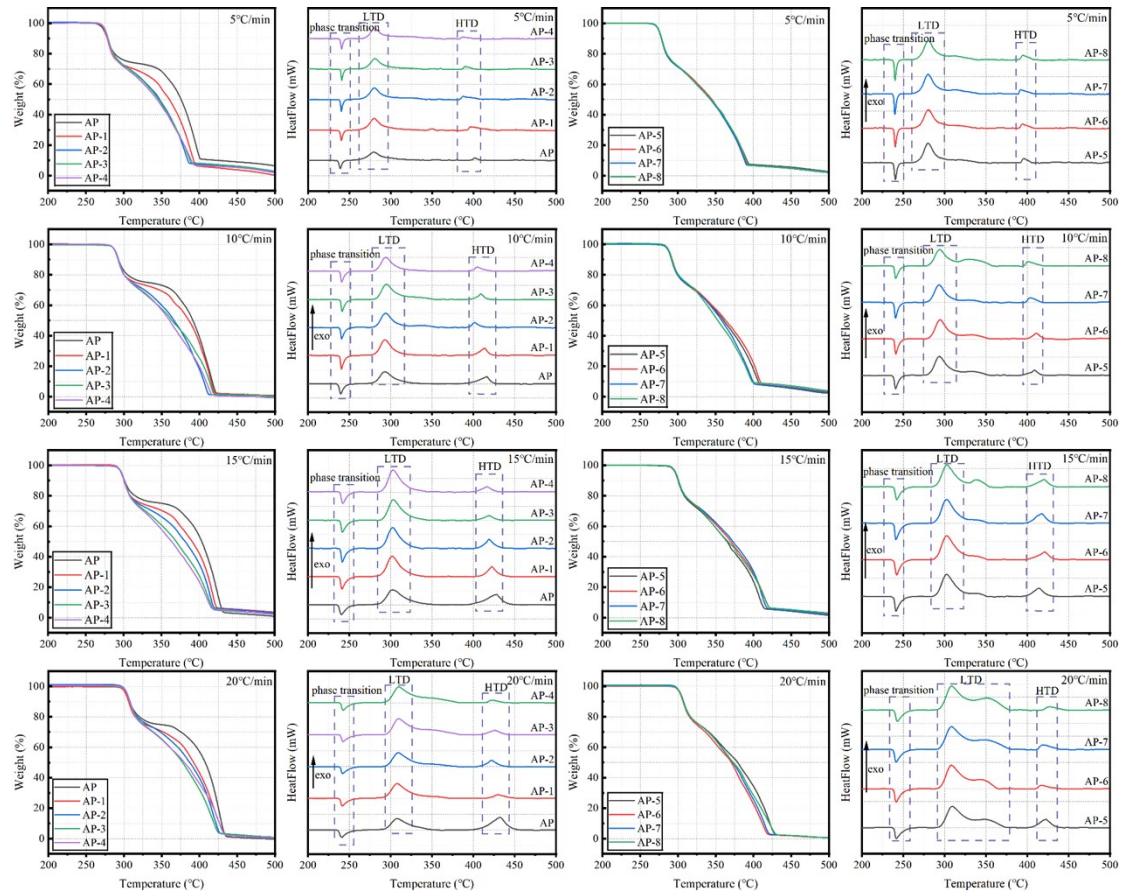


Figure S6. Thermal analysis of AP-based energetic microcapsules.

Table S1. Linear fitting formula for $\ln(\beta/T_p^2) \sim 1000/T_p$ of AP-based energetic microcapsules.

Sample	Linear fitting equation	R^2
AP	$y = -19.00728x + 16.75819$	0.9932
AP-1	$y = -17.99091x + 15.46039$	0.9965
AP-2	$y = -15.84261x + 12.63712$	0.98055
AP-3	$y = -15.2785x + 11.71153$	0.99378
AP-4	$y = -16.20752x + 13.1872$	0.99421
AP-5	$y = -17.0034x + 14.28432$	0.999
AP-6	$y = -17.35178x + 14.62493$	0.99846
AP-7	$y = -17.49362x + 15.01972$	0.98571
AP-8	$y = -18.05261x + 15.74125$	0.9532

Table S2. Thermodynamic/kinetic parameters of thermal decomposition for AP-based energetic microcapsules.

Sample	E_a kJ/mol	$\ln A$ s^{-1}	$k(T_p)$ s^{-1}	ΔH^\ddagger kJ/mol	ΔS^\ddagger J/mol	ΔG^\ddagger kJ/mol
AP	158.0	22.5	0.0121	152.2	-64.9	198.0
AP-1	149.6	21.2	0.0119	143.7	-76.1	197.2
AP-2	131.7	18.2	0.0104	125.9	-100.5	195.9
AP-3	127.0	17.3	0.0100	121.2	-108.6	197.1
AP-4	134.7	18.8	0.0106	129.0	-95.8	195.5
AP-5	141.4	19.9	0.0119	135.6	-86.3	195.8
AP-6	144.3	20.3	0.0115	138.4	-83.3	196.8
AP-7	145.4	20.7	0.0120	139.7	-79.9	195.3
AP-8	150.1	20.4	0.0122	144.3	-73.7	195.7

Table S3. Flowability data parameters of AP-based energetic microcapsules.

Samples	Angle of repose ($^\circ$)	Shear angle ($^\circ$)	Compressibil ity (%)	Homogeneity (a.u.)	Flow index (a.u.)
AP	23.11	25.57	12.00	9.70	88.00
AP-1	32.00	27.44	14.00	9.31	84.00
AP-2	33.29	28.50	14.00	9.62	84.00
AP-3	32.61	29.36	14.00	9.77	84.00
AP-4	30.64	29.08	14.00	9.67	85.00
AP-5	29.27	28.35	12.00	7.70	87.50
AP-6	26.41	27.91	13.00	7.45	89.00
AP-7	33.11	27.88	12.00	7.32	86.00
AP-8	35.32	29.06	10.00	7.13	86.00

Table S4. Jet-ability data parameters of AP-based energetic microcapsules.

Samples	Flow	Angle of	Angle of	Dispersibility	Jet
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	index(a.u.)	rupture (°)	difference (°)	(%)	Index (a.u.)
AP	88.00	21.88	1.23	4.33	52.00
AP-1	84.00	24.69	7.31	3.33	54.52
AP-2	84.00	25.02	8.27	1.67	55.50
AP-3	84.00	24.31	8.30	2.67	56.00
AP-4	85.00	23.56	7.05	2.33	55.25
AP-5	87.50	24.41	4.86	6.67	54.00
AP-6	89.00	22.61	3.80	5.67	52.00
AP-7	86.00	24.68	8.43	3.67	56.00
AP-8	86.00	25.44	9.85	2.67	57.00
