Supplementary Information

Fabrication of Ammonium Dinitramide/Si Energetic Coparticles from Silicon Waste with Enhanced Combustion Heat and Ignition Performance

Chenxi Qu [ab], Qian Liu [b], Jianhua Bu [b], Kewei Ding*[b], Songsong Guo [b], Na Li [b], Hexin Liu[b], Hansheng Li [a], Jian Lv [b]

[a] *School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing 100081, China.*

[b] *Xi'an Modern Chemistry Research Institute, Xi'an 710065, China. Email: dkw204@163.com*

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Preparation of ADN/Silicon waste composites

Materials

Photovoltaic silicon kerf waste powder (RSi) was provided by Sichuan Yongxiang Photovoltaic Technology Co., Ltd. Leshan, China. Silicon carbide (SiC) powder (500–800 mesh) and Fe-containing alloy powder (spherical 316L stainless steel) were provided by Zhongmai Metal Materials Co., Ltd. (Shijiazhuang, China). All other reagents used in this section were consistent with those described for the commercial silicon powder system.

Composite Preparation

The silicon surface pretreatment protocol and the fabrication procedure of ADN/RSi composite samples were identical to those established for commercial silicon powder-based ADN/Si composites. Briefly, ADN/RSi composites with a fixed ADN mass fraction of 80% were first prepared via the solution infiltration and solvent evaporation method described above. Subsequently, SiC powder and 316L stainless steel powder were separately doped into the as-prepared ADN/RSi-80 composite at a mass fraction of 5%, yielding the impurity-containing ADN/RSi-SiC and ADN/RSi-Fe samples, respectively.

The characterization methodologies and performance testing protocols for all ADN/RSi series samples were fully consistent with those applied to the aforementioned ADN/Si composite samples.

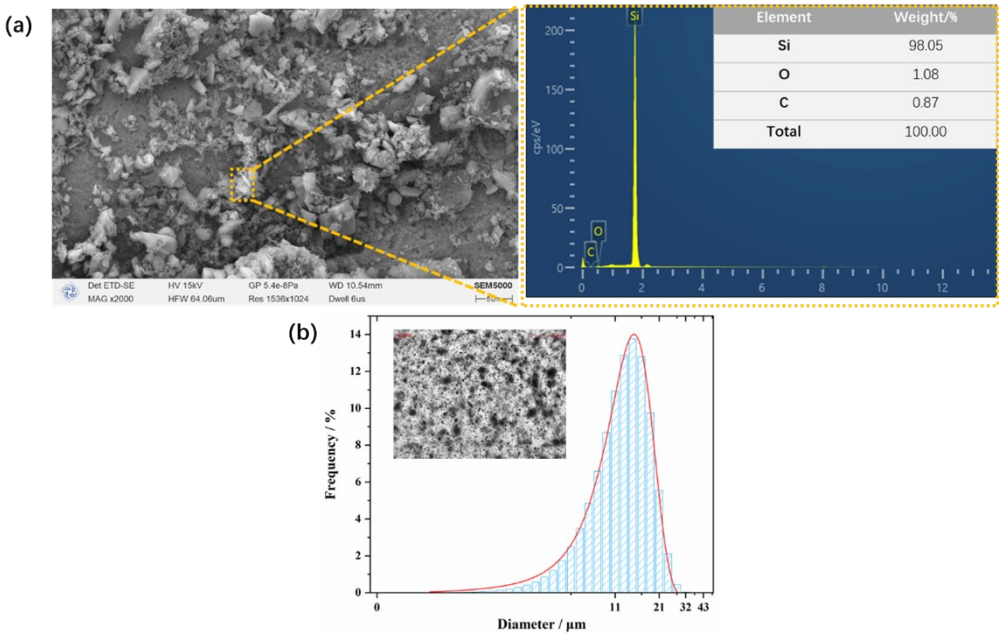


Figure S1. (a) SEM images and EDS analysis of RSi; (b) Particle size distribution of RSi

Particle size distribution analysis of silicon waste samples was performed using an Online 2D Imaging Probe (Pharmavision (Qingdao) Intelligent Technology Co., Ltd.). 500 mg of RSi sample was dispersed in 100 mL of ethanol solution. Images were acquired at a rate of 30 fps, with synchronous capture of static photographic images, and the corresponding particle size distribution data were collected.

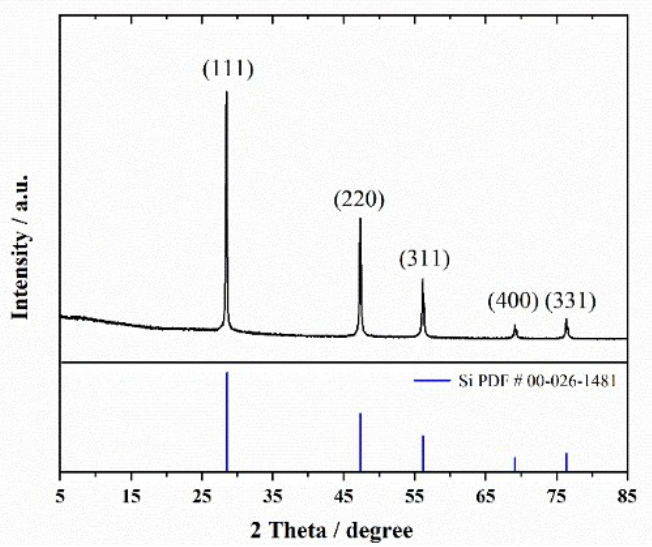
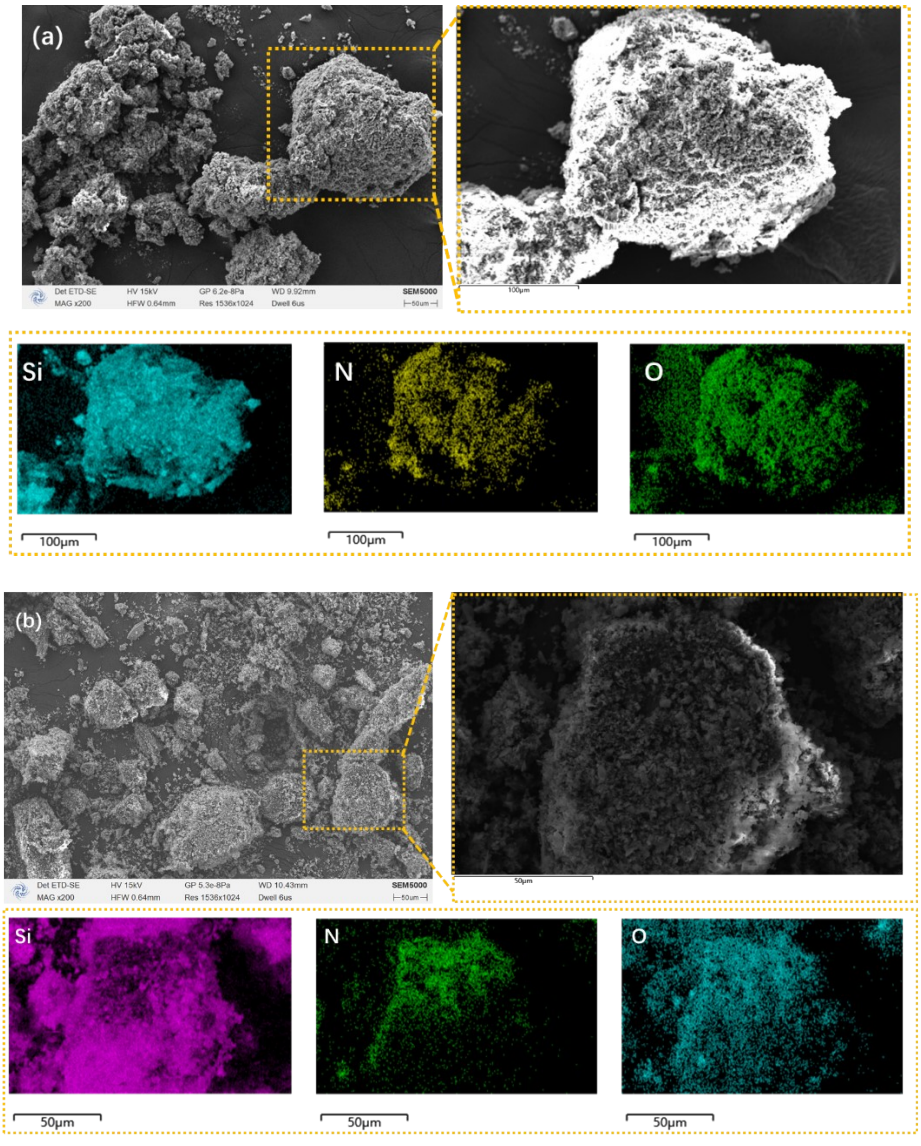


Figure S2. XRD patterns of RSi



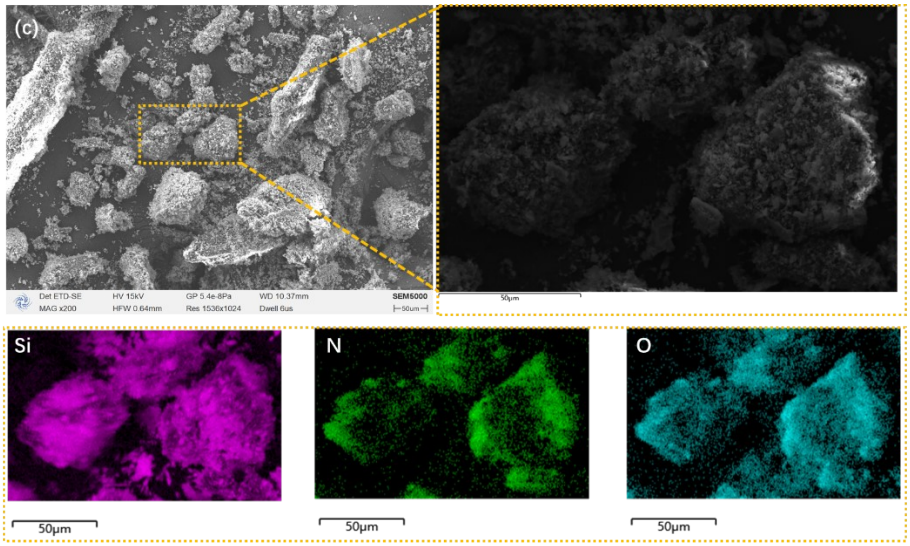


Figure S3. SEM images and EDS analysis of (a) ADN/RSi-30, (b) ADN/RSi-50 and (c) ADN/RSi-80

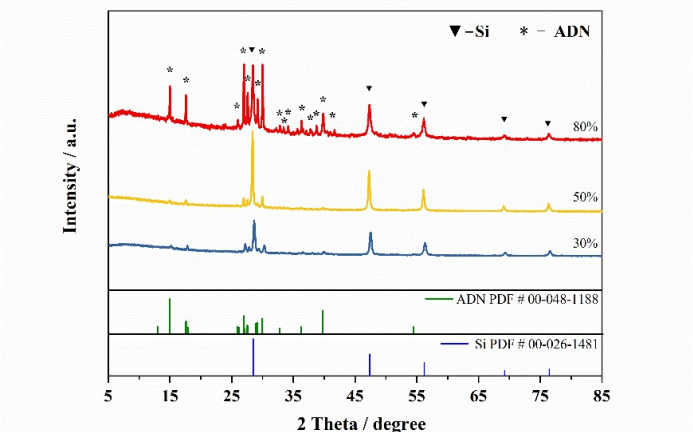


Figure S4. XRD patterns of ADN/RSi coparticles

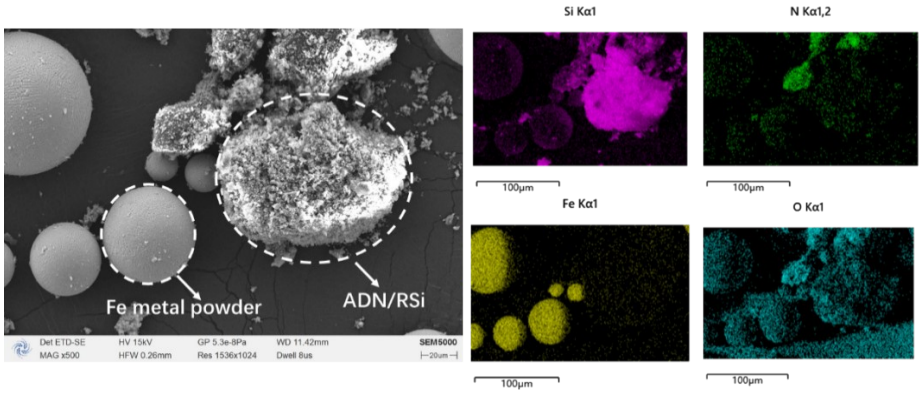


Figure S5. SEM images and EDS analysis of ADN/RSi-Fe

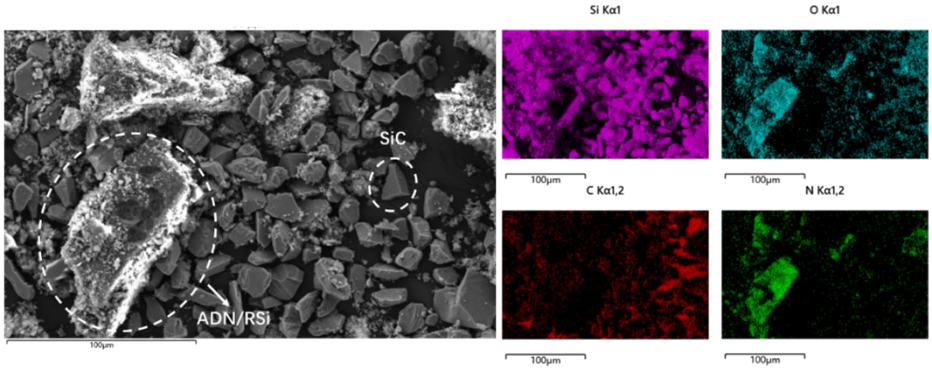


Figure S6. SEM images and EDS analysis of ADN/RSi-SiC

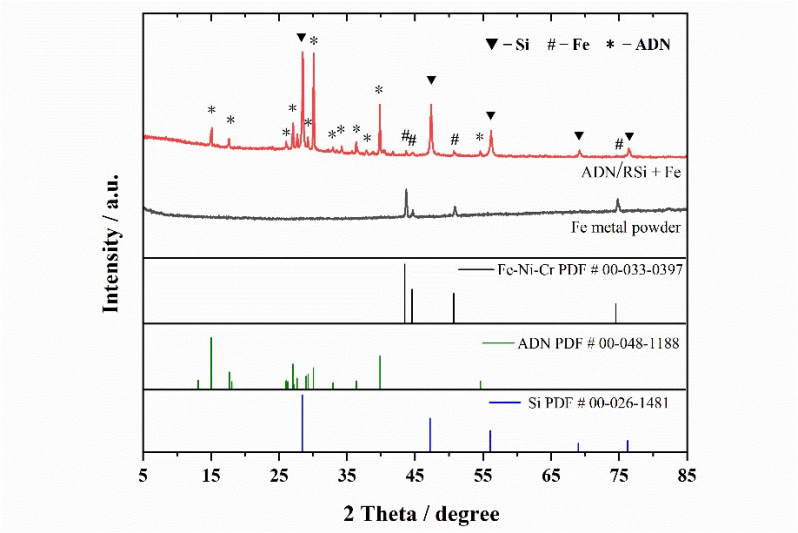


Figure S7. XRD patterns of ADN/RSi-Fe sample

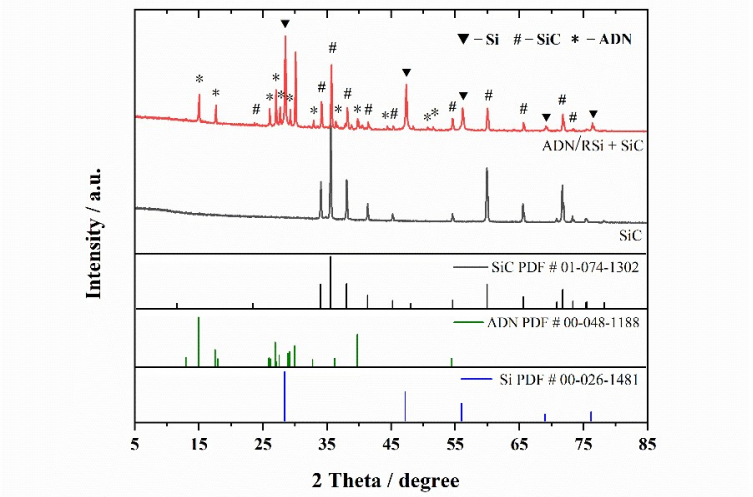


Figure S8. XRD patterns of ADN/RSi-SiC sample

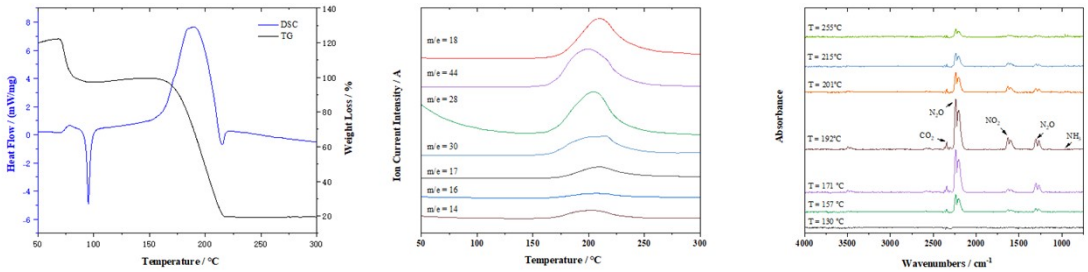


Figure S9. TG-DSC-MS-FTIR analysis of ADN/RSi-80

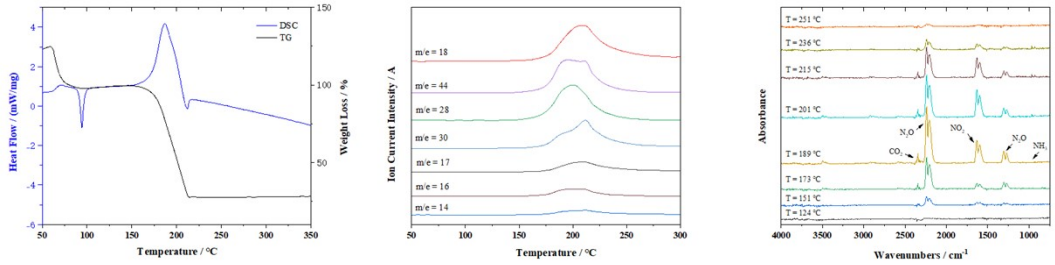


Figure S10. TG-DSC-MS-FTIR analysis of 5%wt ADN/RSi-Fe

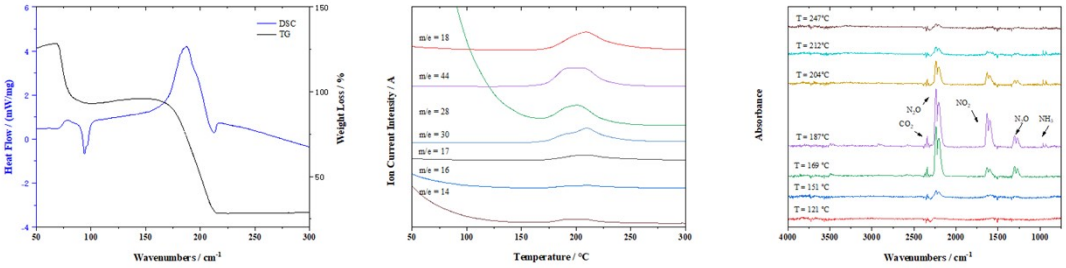


Figure S11. TG-DSC-MS-FTIR analysis of 5%wt ADN/RSi-SiC

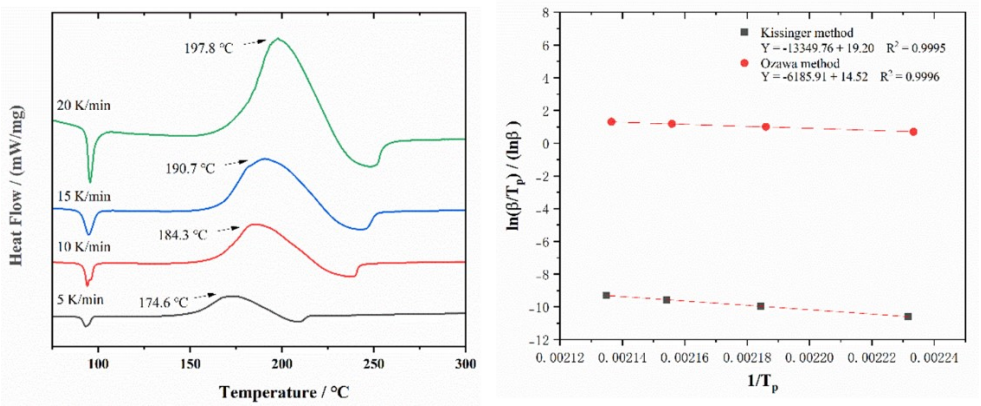


Figure S12. DSC curves and Linear fitting plots of ADN/RSi-80 at different heating rates (5, 10, 15, and 20 K/min)

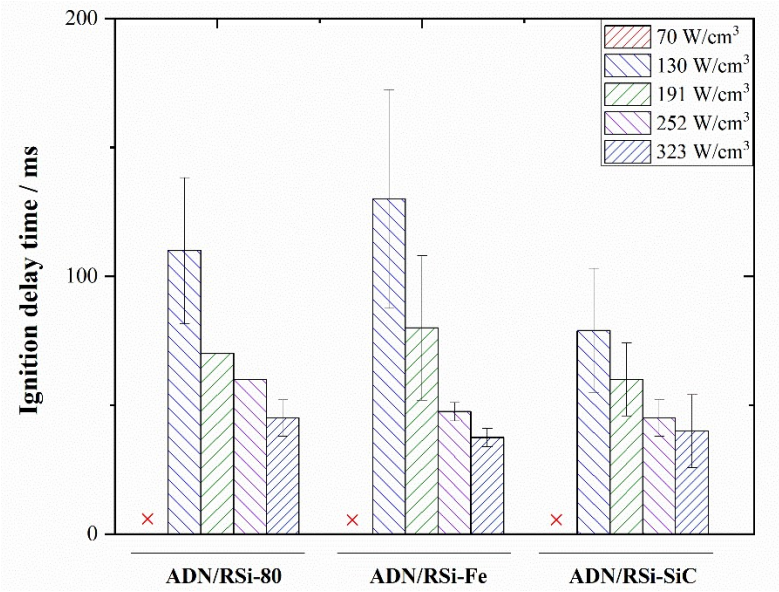


Figure S13. Laser ignition delay times of ADN/RSi, ADN/RSi-Fe and ADN/RSi-SiC composites

Table S1. ICP-MS Detection Results of Elements in RSi Sample

Element	Monitored m/z	Sample Mass (g)	Dilution Factor	Measured Concentration in Solution (C_0, μg/L)	Elemental Concentration in Sample (C_x, μg/kg)	Mass Fraction (%)
Si	28	0.0527	1000	2094.69	993687.8	0.9937
Al	27	0.3545	10	89.21	62909.11	0.00629
Ca	40	0.3545	1	3220.4	227108.6	0.02271
Fe	56	0.3545	1	127.48	8967	0.000897
Na	23	0.3545	1	1033.56	72888.26	0.00729
K	39	0.3545	1	512.5	36142.23	0.00361
Mg	24	0.3545	1	602.76	42507.66	0.00425
S	32	0.0527	1	0.28	131.12	0.00013
B	11	0.3545	1	71.12	5015.76	5.02×10^{-6}
P	31	0.3545	1	238.36	16828.64	1.68×10^{-5}
Pb	208	0.3545	1	38.52	2714.18	2.71×10^{-6}
Ti	48	0.3545	1	67.76	4770.59	4.77×10^{-6}
Zn	66	0.3545	1	1.8	126.4	1.26×10^{-7}
Hg	202	0.3545	1	0.085	5.98	5.98×10^{-9}

Elemental Analysis Methodology for Silicon Sample (ICP-MS)

The elemental analysis of the silicon sample (sample ID: si) was performed using an Agilent 7800 Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) instrument. The flow rates of the carrier gas and auxiliary gas (both high-purity argon, Ar) were 1.00 L/min, and the pump speed was 20 r/min.

For sample pretreatment, the sample mass used for the determination of silicon (Si) and sulfur (S) was 0.0527 g, while 0.3545 g of sample was used for the analysis of other elements. All digested samples were volumetrically made up to 25 mL with ultrapure water. The dilution factors applied were 1000-fold for Si, 10-fold for aluminum (Al), and 1-fold for the remaining elements.

Table S2. Decomposition Kinetic Parameters of ADN/RSi-80 sample

Sample	β (K · min^{-1})	T_p (°C)	E_k (kJ/mol)	lnA (s^{-1})	E_o (kJ/mol)
ADN/RSi-80	5	174.6	111.0 (R^2 = 0.9997)	28.7	112.6 (R^2 = 0.9993)
	10	184.3			
	15	190.7			
	20	195.1			

Table S3. Combustion heat and mechanical sensitivity of ADN/RSi, ADN/RSi+Fe and ADN/RSi+SiC composites

Sample	IS / J	FS / N	Combustion heat / (J/g)
ADN/RSi-30	20	252	5526
ADN/RSi-50	13	144	8673
ADN/RSi-80	6	108	11980
ADN/RSi-Fe	25	96	10889
ADN/RSi-SiC	18	108	11193