Support Information (SI) Appendix

S1. Plastic Spectral Database: Sample and Equipment Details

The Plastic Spectral Database comprises 122 unaged plastic packaging samples from four commonly recyclable plastic types: high-density polyethylene (HDPE), low-density polyethylene (LDPE), polypropylene (PP), and polyethylene terephthalate (PET). The samples, sourced from both purchased products and post-consumer recyclable waste, were identified using Resin Identification Codes (1 for PET, 2 for HDPE,4 for LDPE, 5for PP) when available; otherwise, FTIR spectroscopy was employed. Prior to analysis, all samples were thoroughly cleaned with water and detergent and cut into approximately 30×50 mm pieces for spectroscopic measurements.

The database includes spectral data from three techniques: FTIR, RAMAN, and LIBS.FTIR measurements were conducted using a Thermo Fisher Nicolet iN10 MX infrared microscope with a Germanium micro-tip ATR crystal, covering the range of 675 to 4000 cm–1 with a resolution of 4 cm–1 and 32 scans per sample. For Raman measurements, a Renishaw InVia confocal Raman microscope with a 785 nm laser was used, covering 500 to 3200 cm–1 with a laser power of 30 mW and 10 seconds of acquisition time. This wavelength was selected to minimize fluorescence interference, particularly for PET samples. LIBS measurements were made using a SciAps Z-300 handheld analyzer with a 1064 nm laser, covering 180–700 nm in an argon atmosphere. Spectra were averaged from four measurement points on each sample, with cleaning shots performed between measurements to ensure accurate results.



Fig. S1. (a) Interpolation comparison of FTIR, (b) Interpolation comparison of RAMAN, (c)



Fig. S2. (a) Original spectra, (b) Preprocessed spectra, (c) PCA visualization of original spectra, (d) PCA visualization of preprocessed spectra.



Fig. S3. (a) Original spectra, (b) Preprocessed spectra, (c) PCA visualization of original spectra, (d) PCA visualization of preprocessed spectra.



Fig. S5. PCA loading of LIBS.



Fig. S6. (a) Difference Spectral Comparison of LDPE, (b) Difference Spectral Comparison of HDPE, (c) Difference Spectral Comparison of PP, (d) Difference Spectral Comparison of

PET.



Fig. S7. (a) Difference Spectral Comparison of LDPE, (b) Difference Spectral Comparison of HDPE, (c) Difference Spectral Comparison of PP, (d) Difference Spectral Comparison of PET.



Fig. S8. (a) T-SNE Distribution of LDPE, (b) T-SNE Distribution of HDPE, (c) T-SNE Distribution of PP, (d) T-SNE Distribution of PET.



Fig. S9. (a) T-SNE Distribution of LDPE, (b) T-SNE Distribution of HDPE, (c) T-SNE Distribution of PP, (d) T-SNE Distribution of PET.