

Supporting Information for
**Speciation of sulfur in biochar produced from pyrolysis and gasification of oak and
corn stover**

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Summary

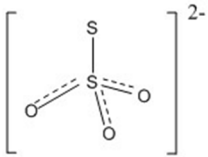
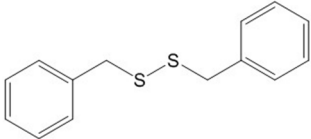
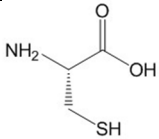
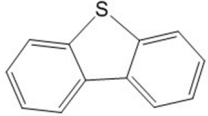
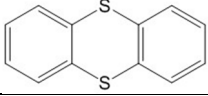
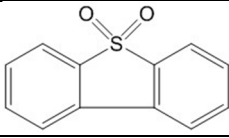
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Table S1. Model compounds used in this study.

Figure S1. XANES spectra of model compounds.

Figure S3. X-ray diffraction patterns of the biochars.

Table S1. Model compounds used in this study. The values of the white lines were obtained from derivatives of the respective spectra.

Model compound	Structural formula	White line (eV)
Ni ₃ S ₂		2471.43
NiS		2471.47
Thiosulfate (Na ₂ S ₂ O ₃)		2472.02
Dibenzyldisulfide		2472.79
L-cysteine		2473.45
Dibenzothiophene		2473.89
Thianthrene		2474.38
Na ₂ SO ₃		2478.44
Dibenzothiophene sulfone		2479.87
CaSO ₄		2482.70

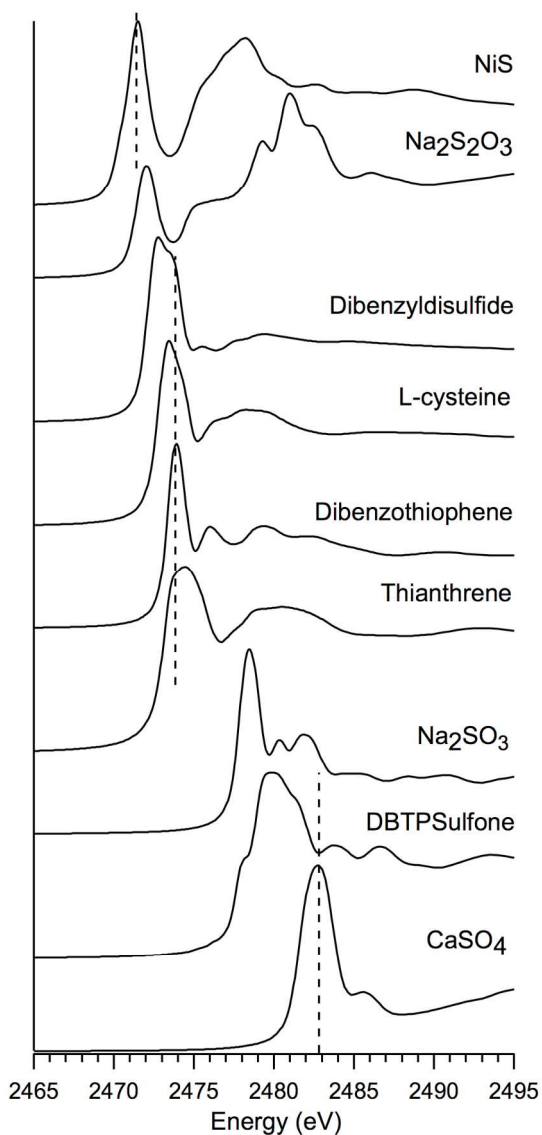


Figure S1. XANES spectra of model compounds. As the oxidation state of sulfur in the molecule or crystal increases, the white line or absorption edge of the sulfur increases. For example, the spectrum of sulfate, the most highly oxidized sulfur species, has an absorption at 2482.70 eV, while the spectrum of NiS has its white line at 2471.47 (indicated by dashed line on the far left). Several of the organic model compounds, L-cysteine, dibenzothiophene, and thianthrene, have absorption peaks that are close to each other in energy (dashed line at approximately 2474 eV, exact values are in Table S1).

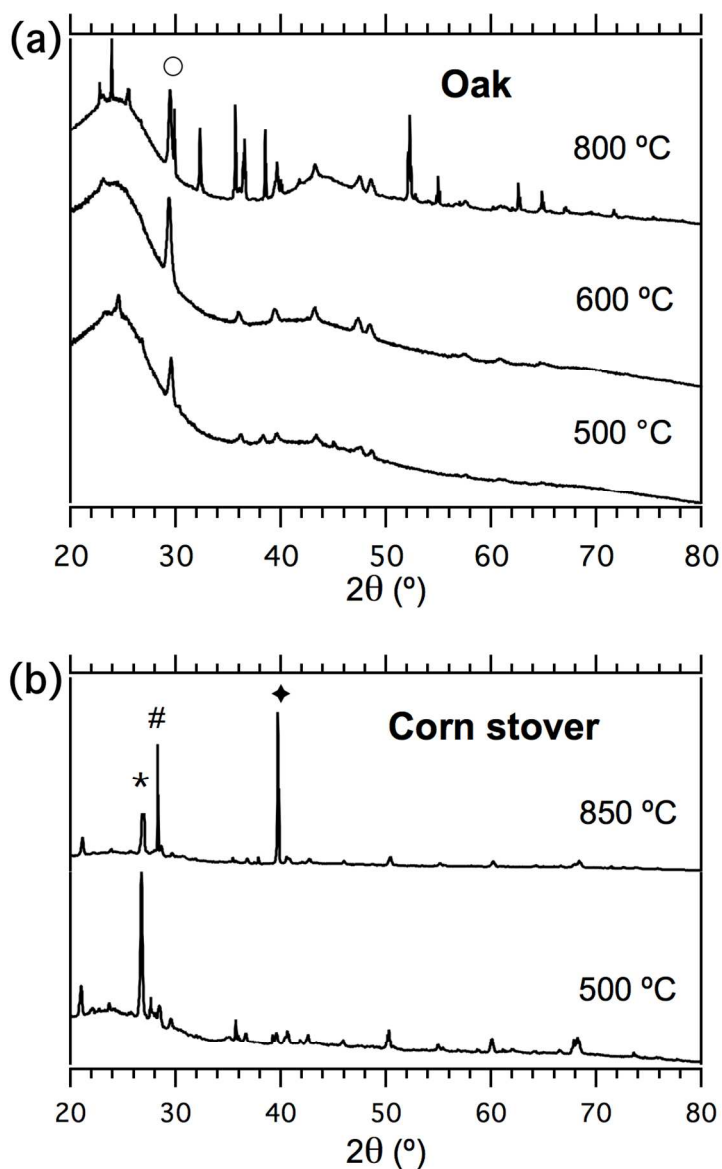


Figure S2. X-ray diffraction patterns of the biochars. The most prominent lines for crystalline minerals in the biochars are marked. In Figure 2(a), the peaks that are unmarked are from olivine reflections; the peak marked with the ○ symbol is from CaCO_3 . In Figure 2(b), the peak marked with the * and # symbols are definitively assigned to SiO_2 and KCl , respectively. The peak marked with the ◆ symbol is consistent with that of CaSiO_3 .