Cyanamide Functionalized Carbon Nitride Semiconductors for Solar Light Driven Fuel Generation

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Introduction

- Photocatalysts can carry out redox reactions using electrons excited by the absorption of the energy of a photon of light exposed to light
- One such photocatalytic material is Melon (C_3N_4), an amorphous polymeric Carbon Nitride
- Poly(heptazine imide) aka PHI, is one form of melon. It can both absorb light to generate excited electrons and store charge. This material can absorb energy from light and store it for later use.
- Potassium(K) is added to balance the negative charge build up forming (K-PHI).

Hypothesis

This material, K-PHI, can extend charge carrier lifetimes when used in heterojunction with Black Phosphorous.

Methodology

- First melon was synthesized by pyrolyzing melamine at 550 degrees Celsius for 12 hours with a ramp of 5 degrees per minute
- K-PHI was synthesized by grinding melon(s, 1.5g) and KSCN(s, 3.0g) together and pyrolyzing at 400 degrees Celsius for 1 hour and then 500 degrees Celsius for 30 minutes
- The product was washed multiple times with deionized water to remove KSCN
- The materials were characterized using diffuse reflectance UV vis spectroscopy, X-ray diffraction(XRD), X-ray photoelectron Spectroscopy(XPS), and FT-IR spectroscopy.

Bigger Picture

- A photocatalyst called Black phosphorous can convert water to hydrogen(H_2)
- The K-PHI photocatalyst studied in this project can generate CO from CO_2 with CO^{2+} sites.
- These products can be used to produce viable fuels via a known process called Fischer-Tropsch
- Because CO_2 and water are products of Fossil Fuel combustion, this material could close the gap in renewability.

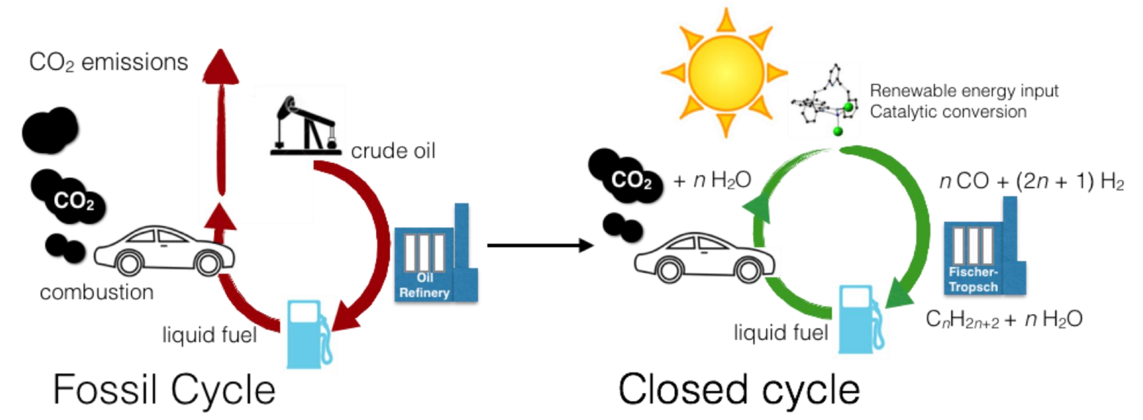
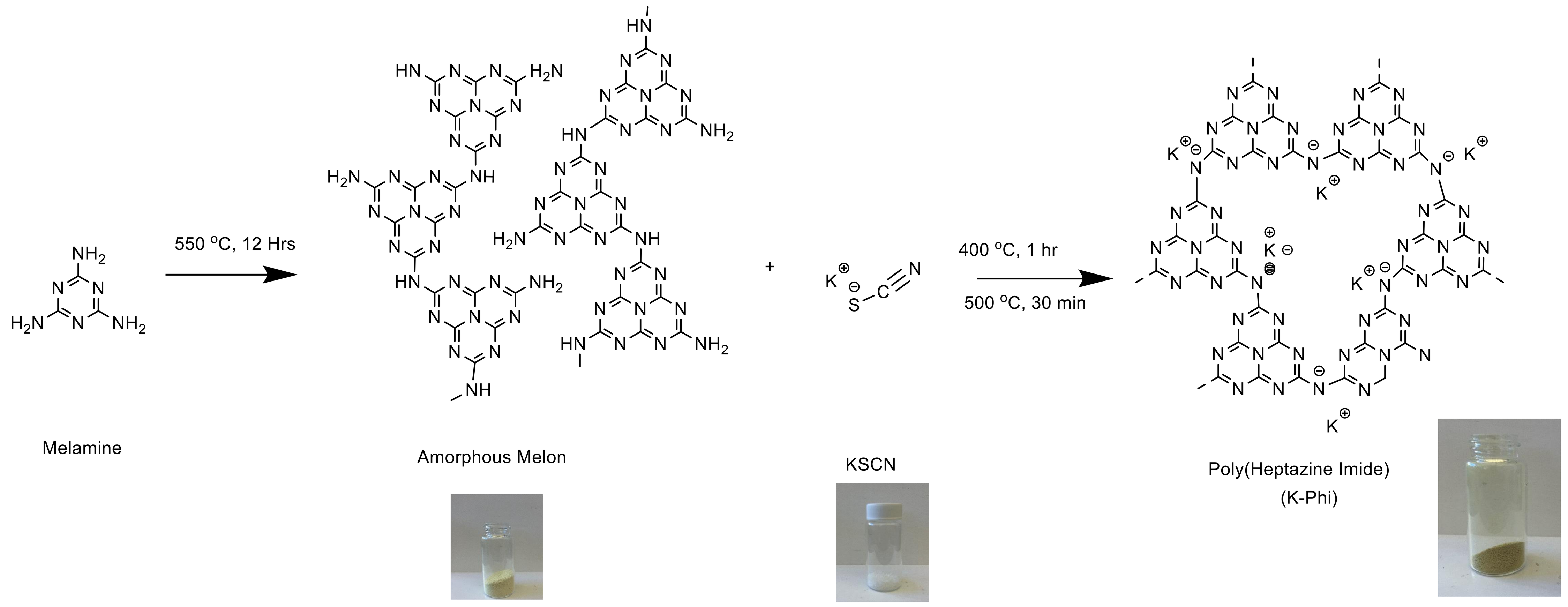


Figure 1: The Fossil fuel cycle in combination with a renewable cycle made possible by photocatalysis.

Reactions



Synthesis and Characterization

Amorphous Melon and KSCN

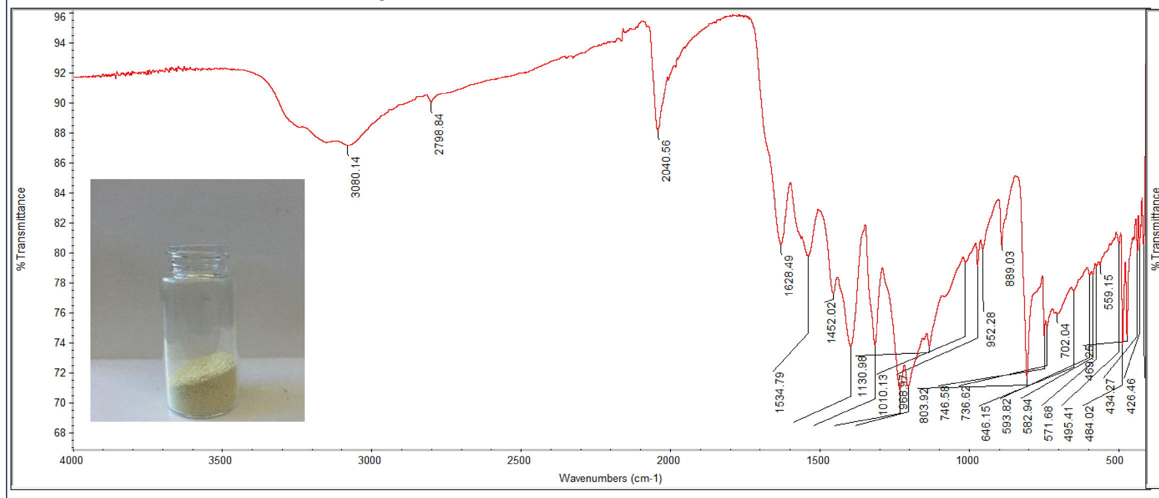


Figure 2: FTIR Spectrum of KSCN and Melon

Poly(Heptazine Imide) aka K-PHI

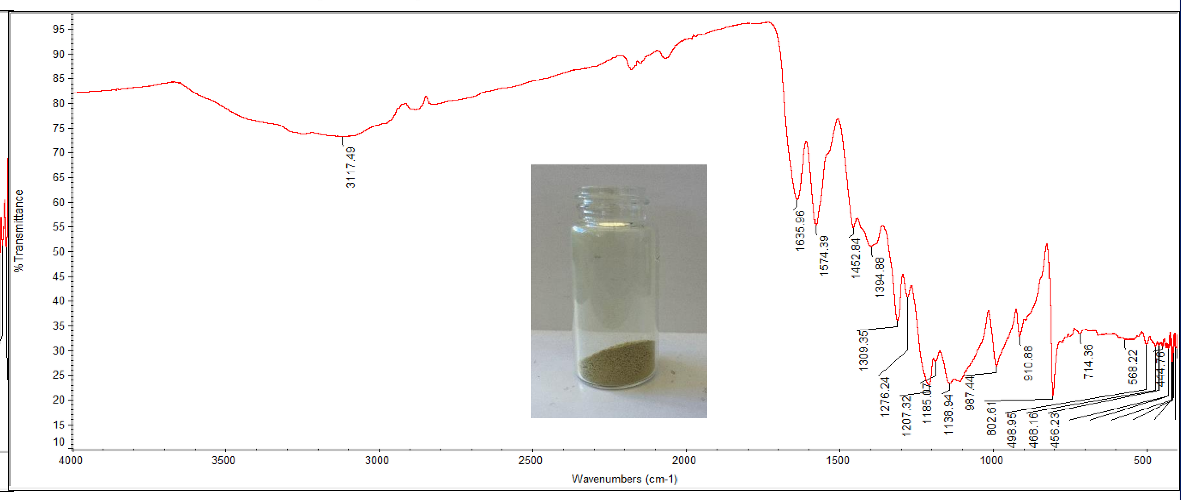


Figure 3: FTIR Spectrum of K-PHI

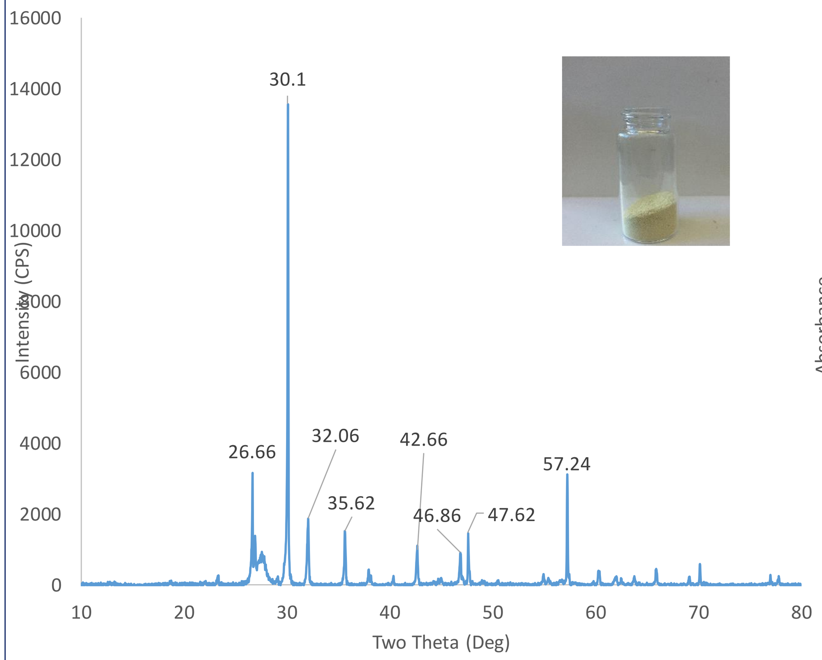


Figure 4: XRD Spectra of KSCN and Melon

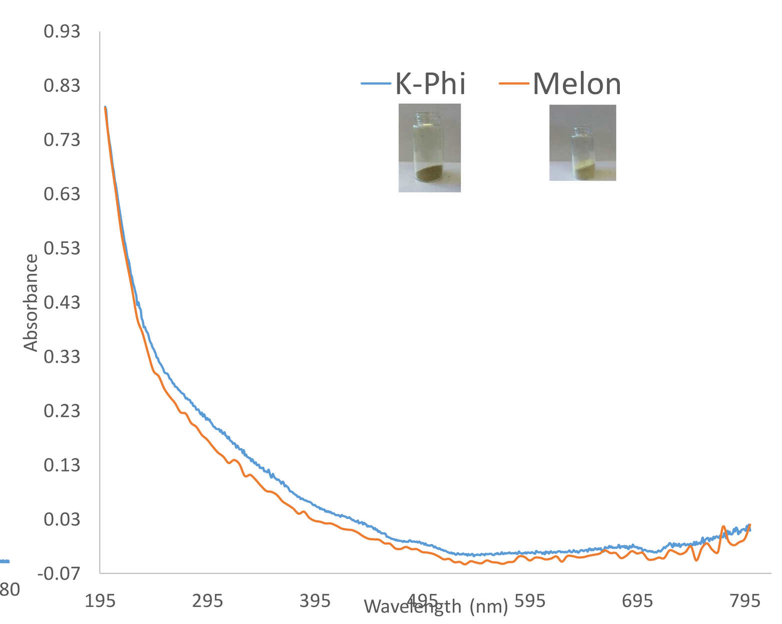


Figure 5: UV Vis Spectrum of both KSCN/Melon and K-PHI

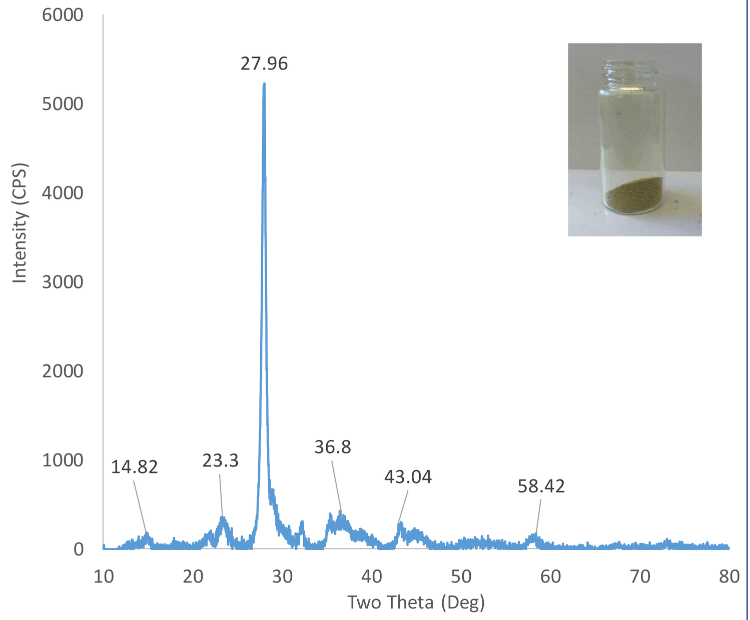


Figure 6: XRD Spectra of K-PHI

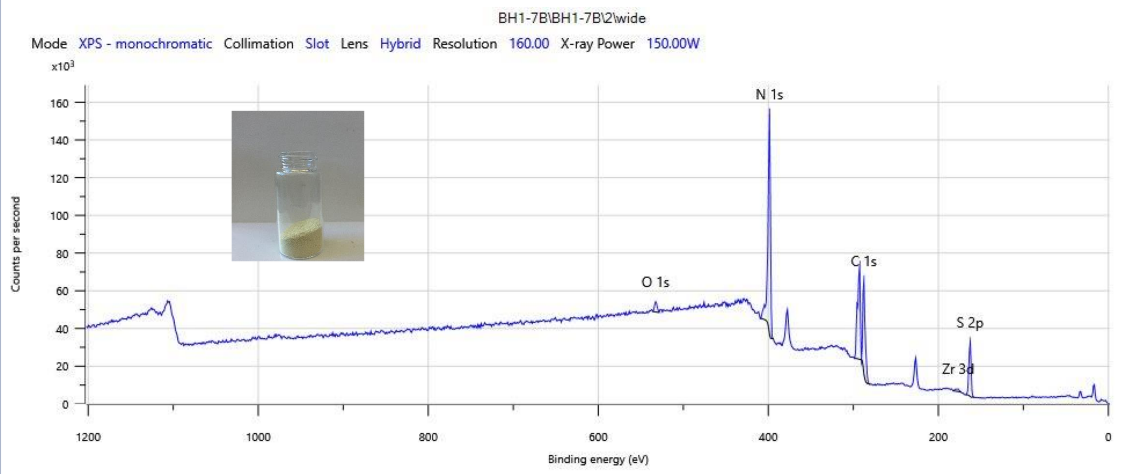


Figure 7: XPS Spectra of KSCN and Melon

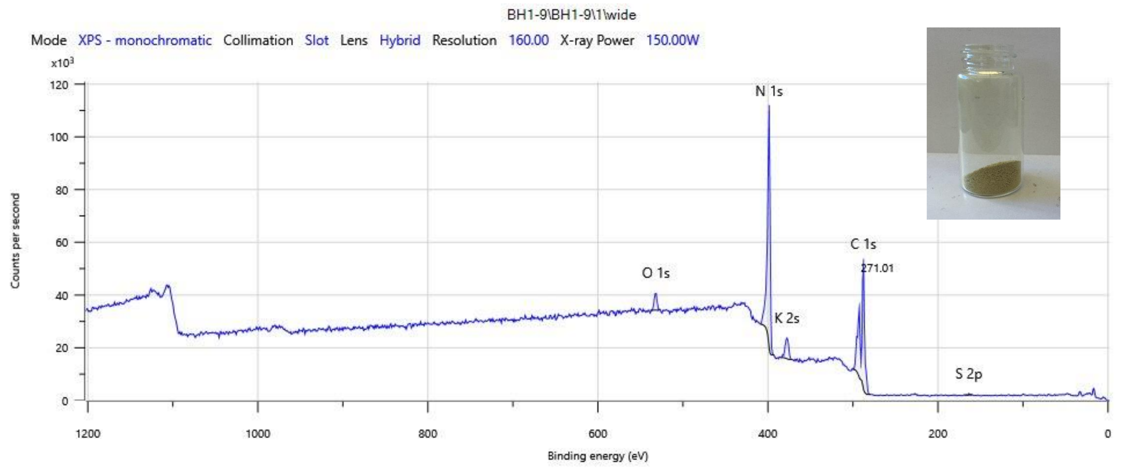


Figure 8: XPS Spectra of K-PHI

Analysis of Figures

FTIR Spectroscopy:

- Both spectra display a broad peak around 3200 wavenumber which is indicative of an N-H bond.
- A peak at 2040 wavenumber on the Melon/KSCN spectra is indicative of a carbon bonded to a sulfur and triple bonded to a nitrogen. This is likely from KSCN. Its absence in the K-PHI shows that the product was pure.

UV Vis Spectroscopy:

- K-PHI has higher absorbance at lower wavelengths. This could be related to the color difference.

X-Ray Diffraction:

- Spectra for K-PHI strongly agrees with other spectra in literature sources. Intense peak at 27 degrees.
- Intense peak at 30 degrees in the spectra for KSCN and Melon agrees with spectra of KSCN. Its absence in K-PHI shows the products purity.

X-Ray Photo electron Spectroscopy:

- Both spectra have peaks which correspond to electrons in the 1s configuration in Carbon and Nitrogen atoms.
- Both spectra show Potassium(K) electrons in the 2s configuration(peaks around 425 eV). However K-PHI yielded a smaller peak, highlighting that some of the potassium was removed as impurity.
- A peak around 230 eV corresponds to 2p electrons in sulfur. This peak is found in the reactants and is essentially absent in K-PHI. This shows that unreacted KSCN was removed properly and that the product is pure.

Conclusions

- K-PHI was successfully generated
- This process was relatively easy and cost effective on a small scale

Next Steps

- Performing a Photocatalysis reaction with the synthesized material with added CO^{2+} sites.
- Performing a simultaneous reaction with black phosphorous
- Scaling to proportions that could be used in industry

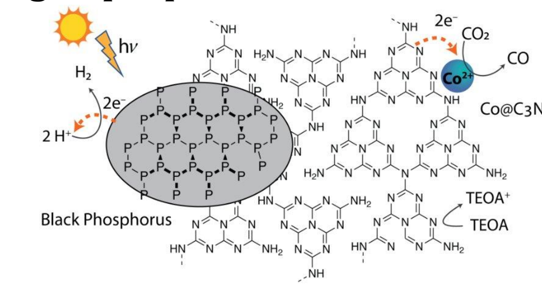


Figure 9: The combination of Black Phosphorous and K-PHI

Acknowledgements

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References

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