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ENGINEERING

“Energy Materials”

Prof. Chris McNeill

Synchrotrons

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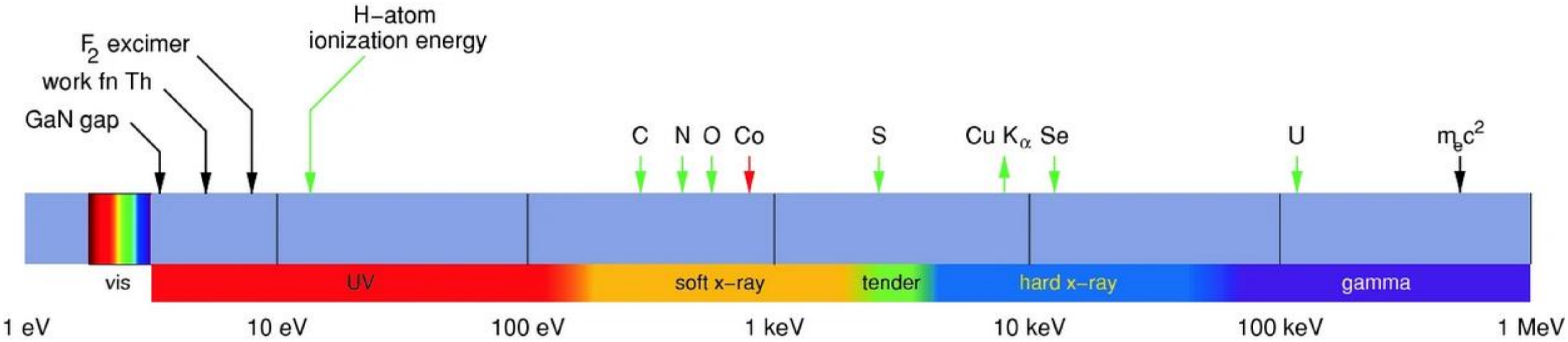
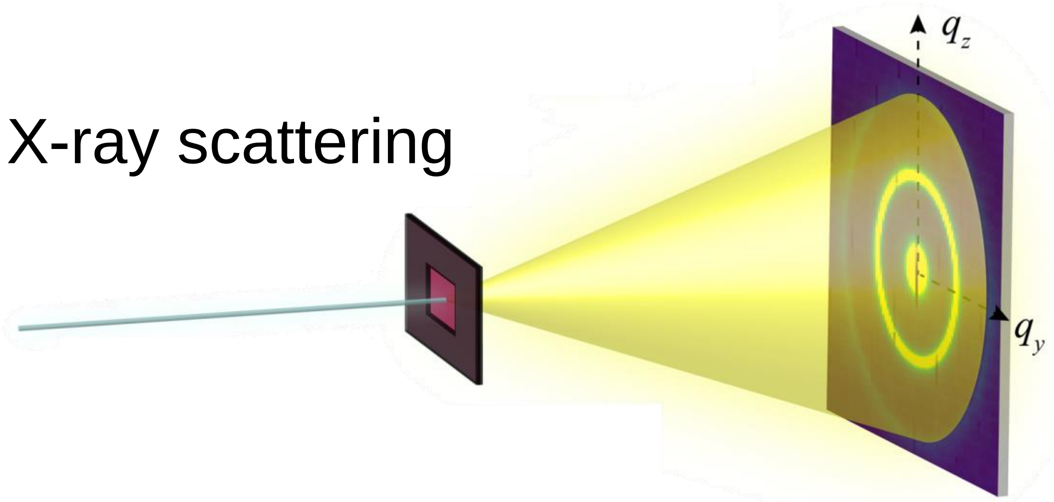
X-rays



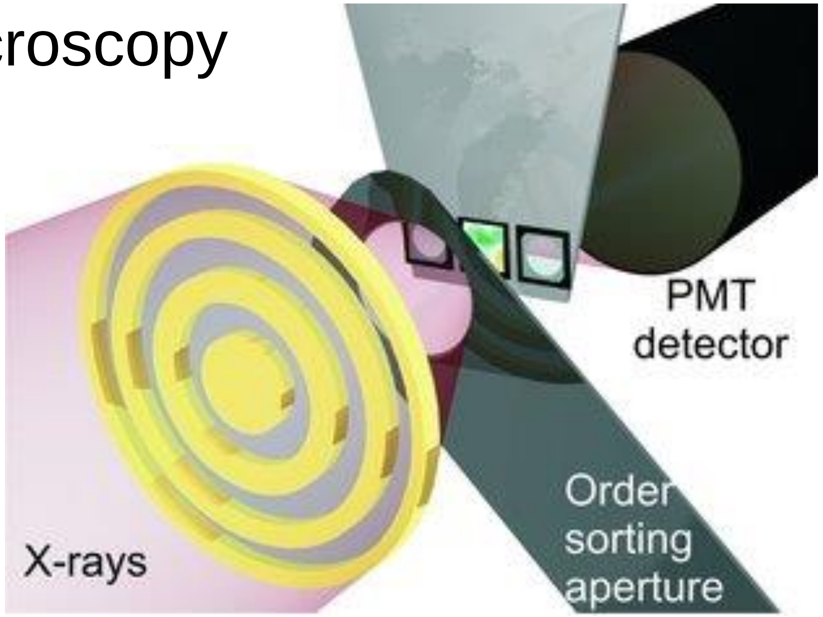
https://doi.org/10.1007/978-3-030-64623-3_1

Techniques

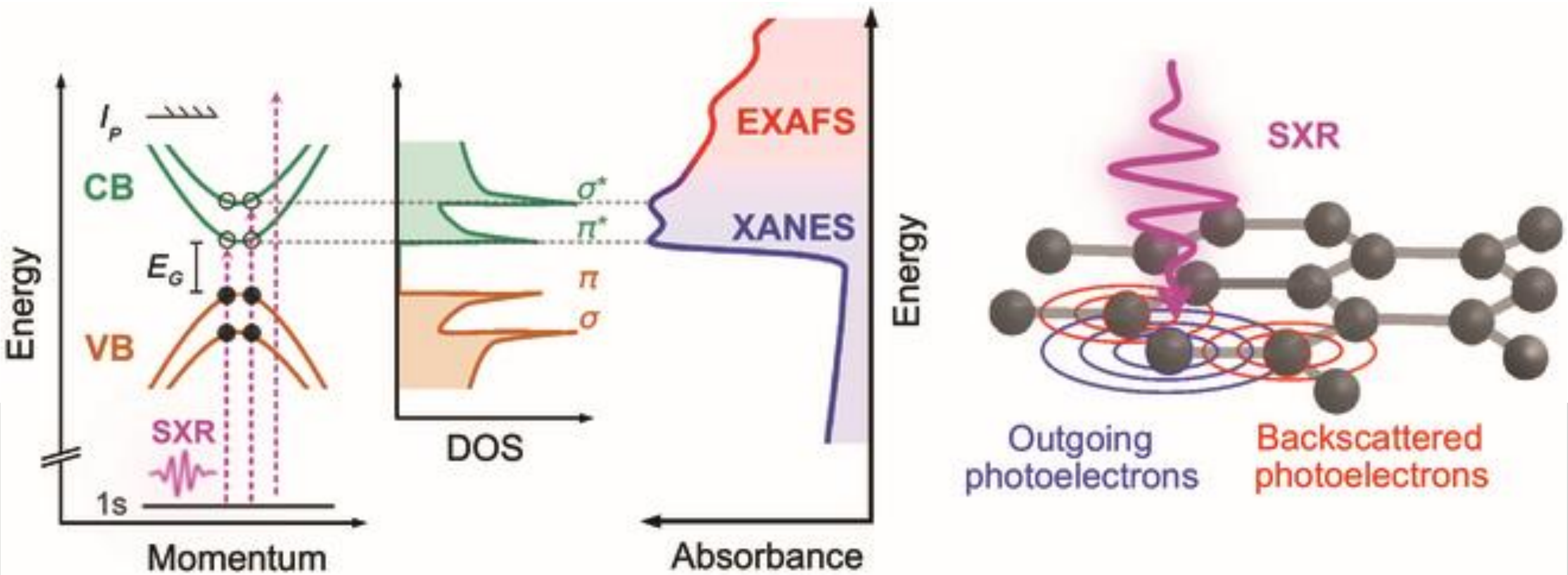
X-ray scattering



X-ray microscopy



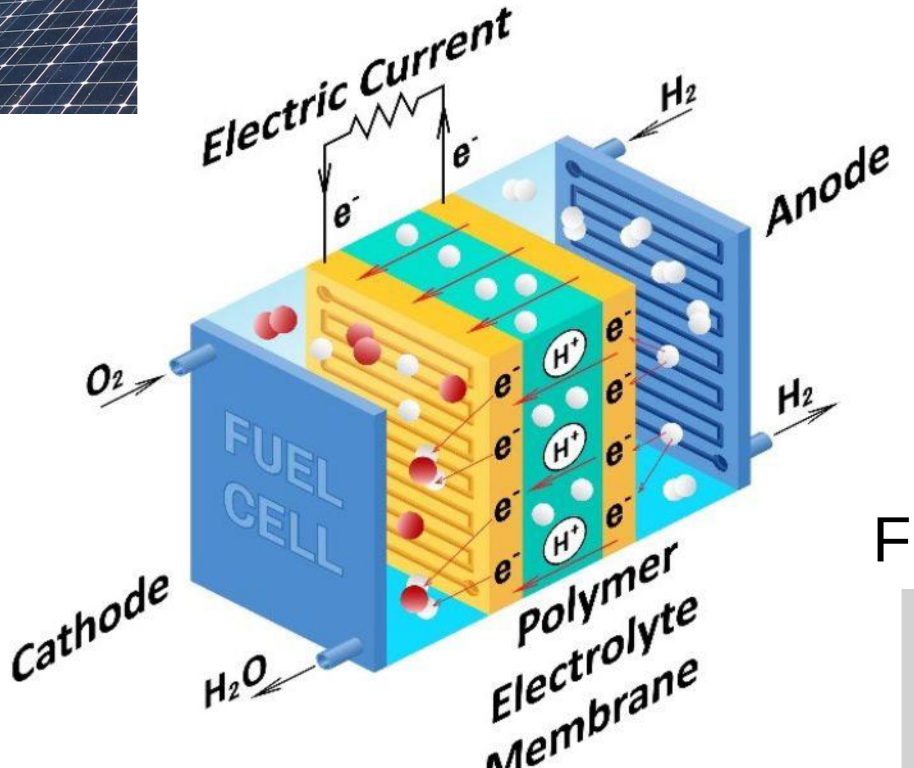
X-ray spectroscopy



Energy Materials

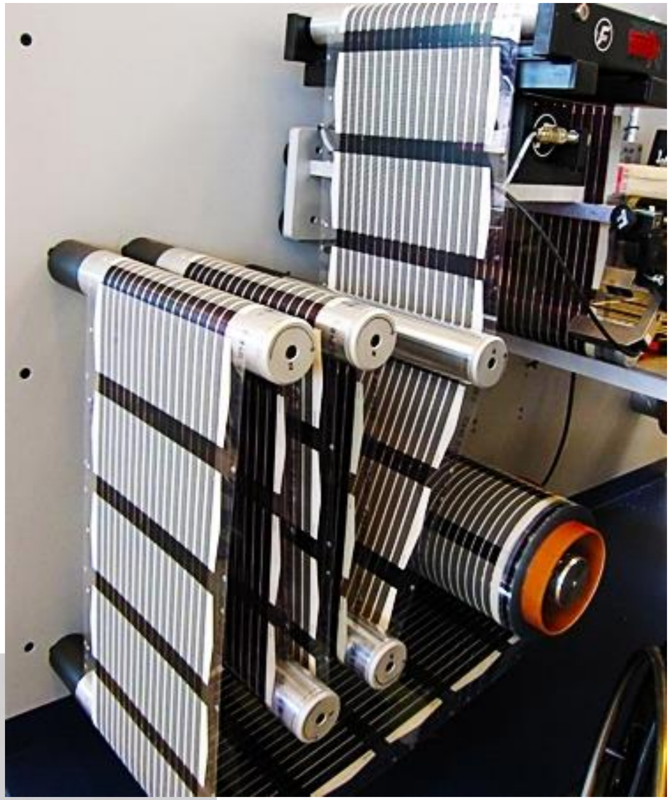
Solar Cells

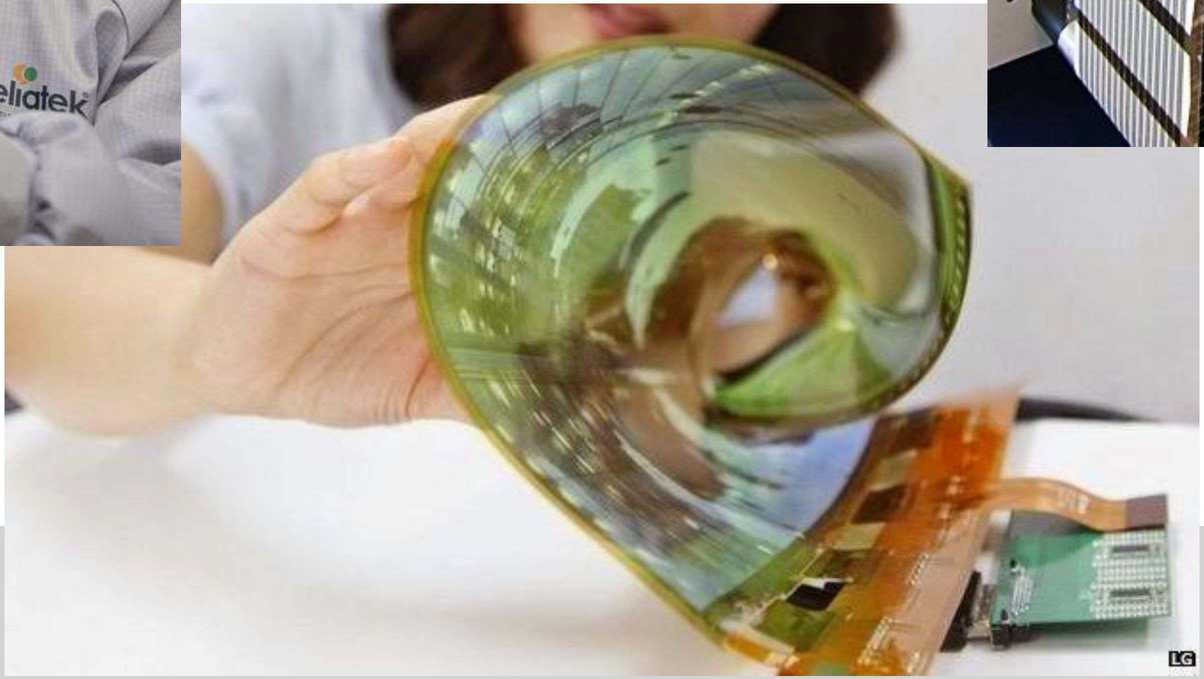
Batteries



Fuel Cells

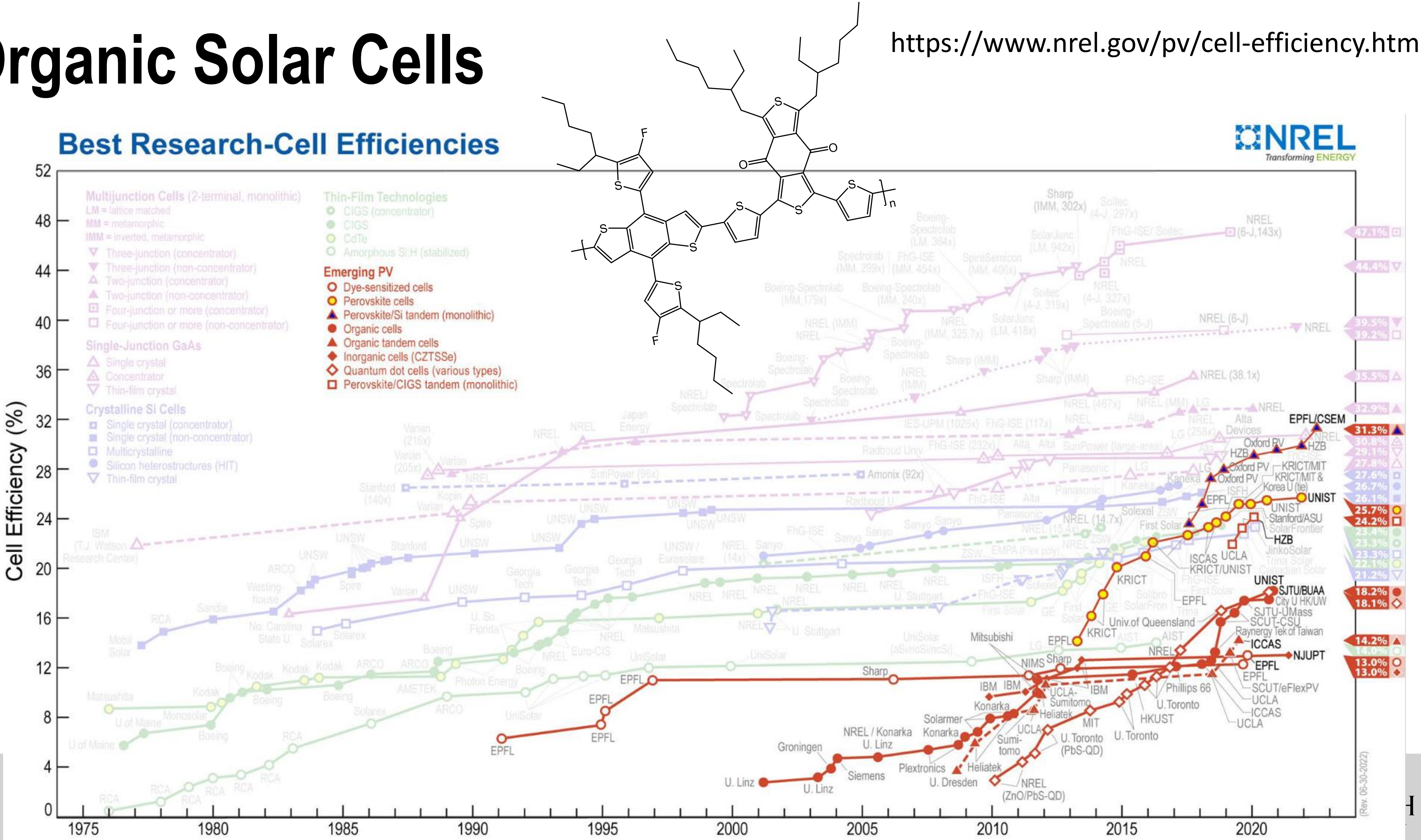
Organic Electronics





Organic Solar Cells

https://www.nrel.gov/pv/cell-efficiency.html

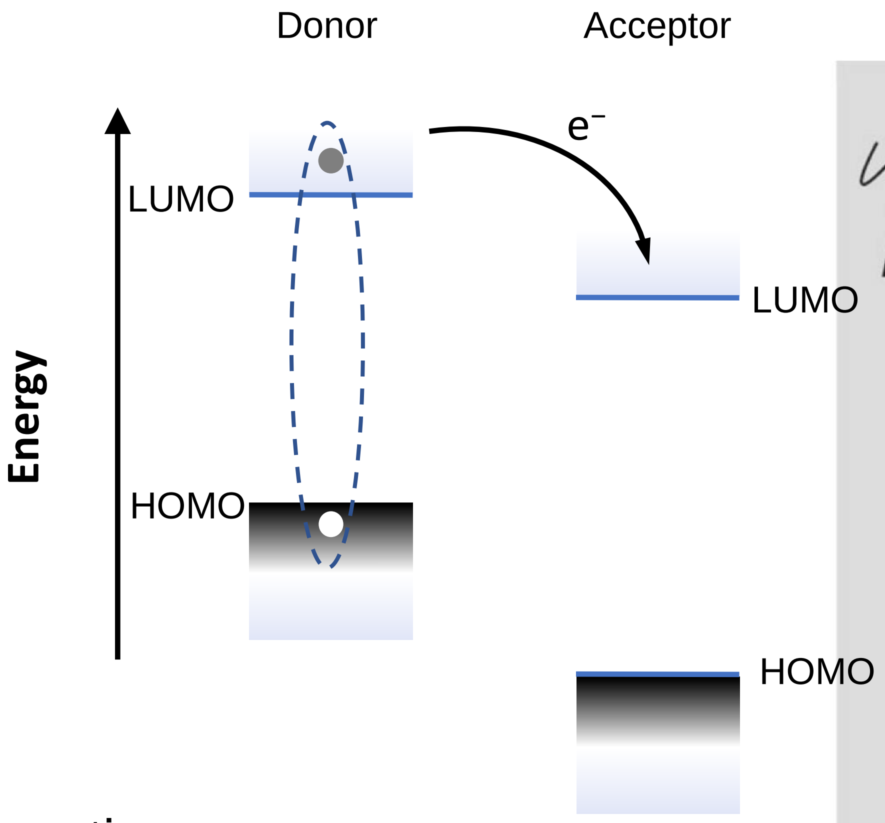


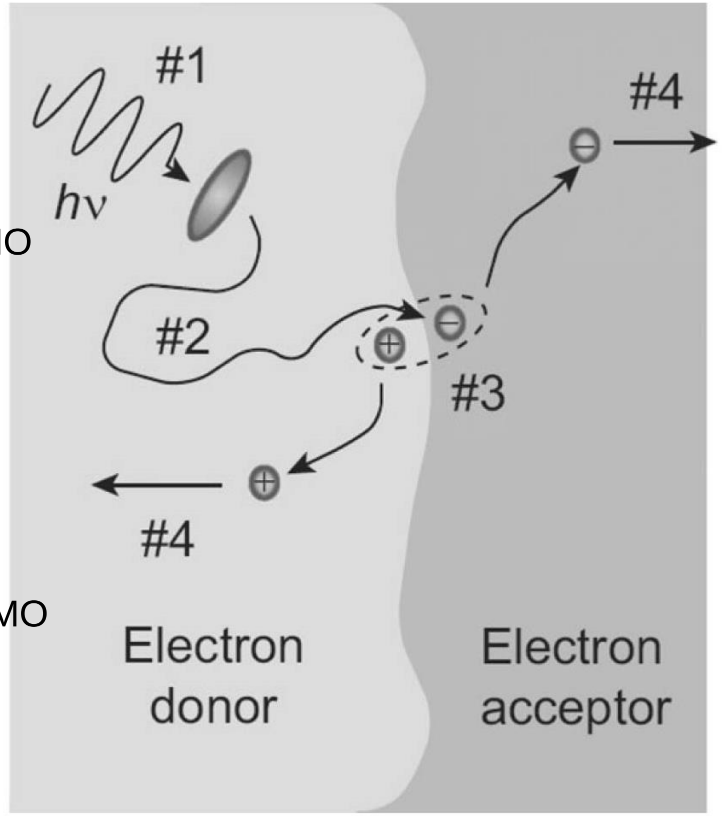
Organic solar cells

Organic semiconductors are strong absorbers of light with readily tunable properties facilitated by organic synthetic chemistry.

Light absorption however leads to the formation of tightly bound excitons with binding energy of ~ 0.4 eV.

Charge generation involves a multi-step process:
Step #1 Light absorption
Step #2 Exciton diffusion to a heterojunction
Step #3 Exciton dissociation at heterojunction
Step #4 Charge separation from heterojunction



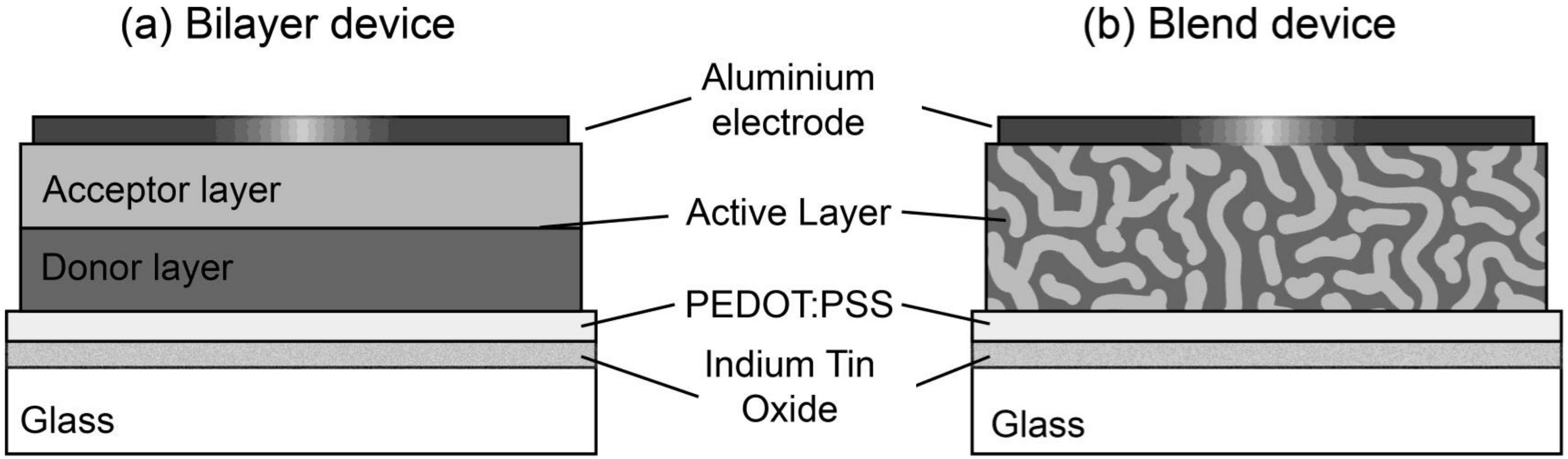


A sufficient difference in the HOMOs and LUMOs of the donor and acceptor materials is required. The “acceptor” has the higher electron affinity (deeper LUMO).

Organic solar cells

Exciton diffusion length is only ~ 10 nm.

Bilayer heterojunction devices not very efficient as we need the layers to be > 100 nm thick.



Solution is the “bulk heterojunction” which is a nanostructured blend of donor and acceptor materials.

Thick enough layers can be produced for good light absorption. Excitons are generated with 10 nm of a heterojunction. Interpenetrating networks allow charges to find the electrodes.

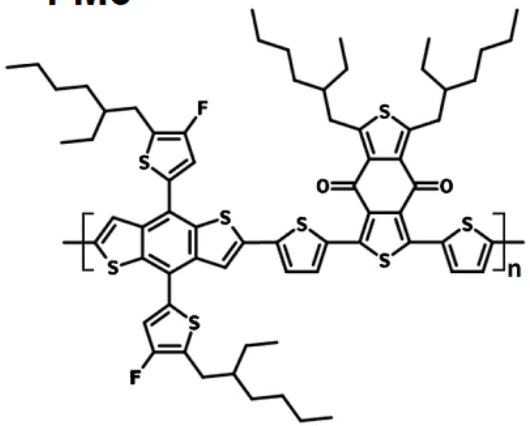
Organic solar cells

Highest efficiency cells use a polymer donor and small molecule acceptor.

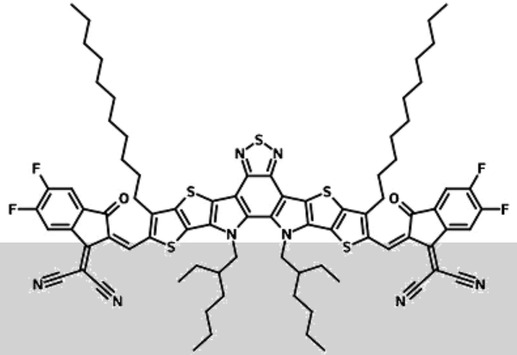
Donor and acceptor have complementary absorption profiles covering the visible to near-IR.

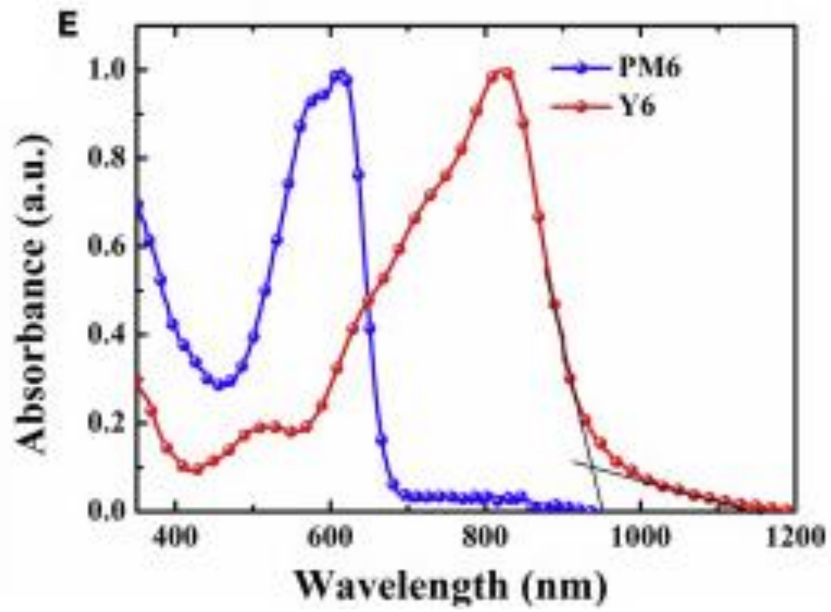
The PM6:Y6 system can achieve efficiencies > 16%

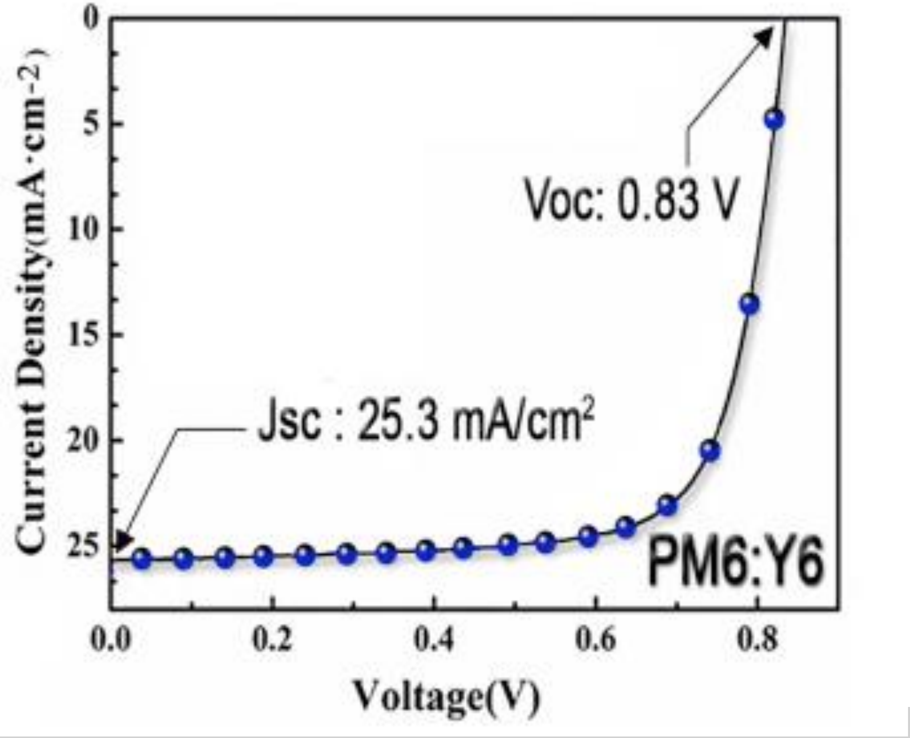
PM6



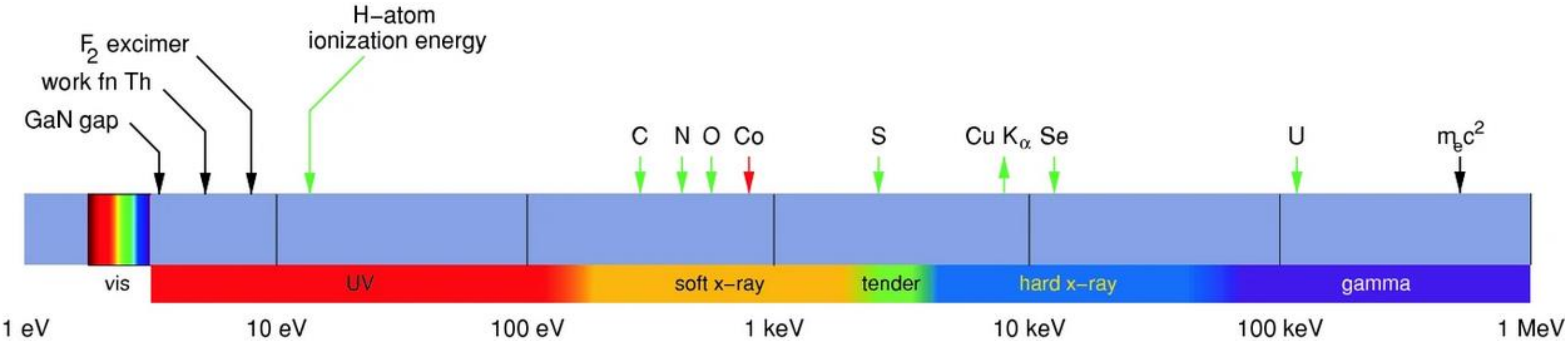
Y6





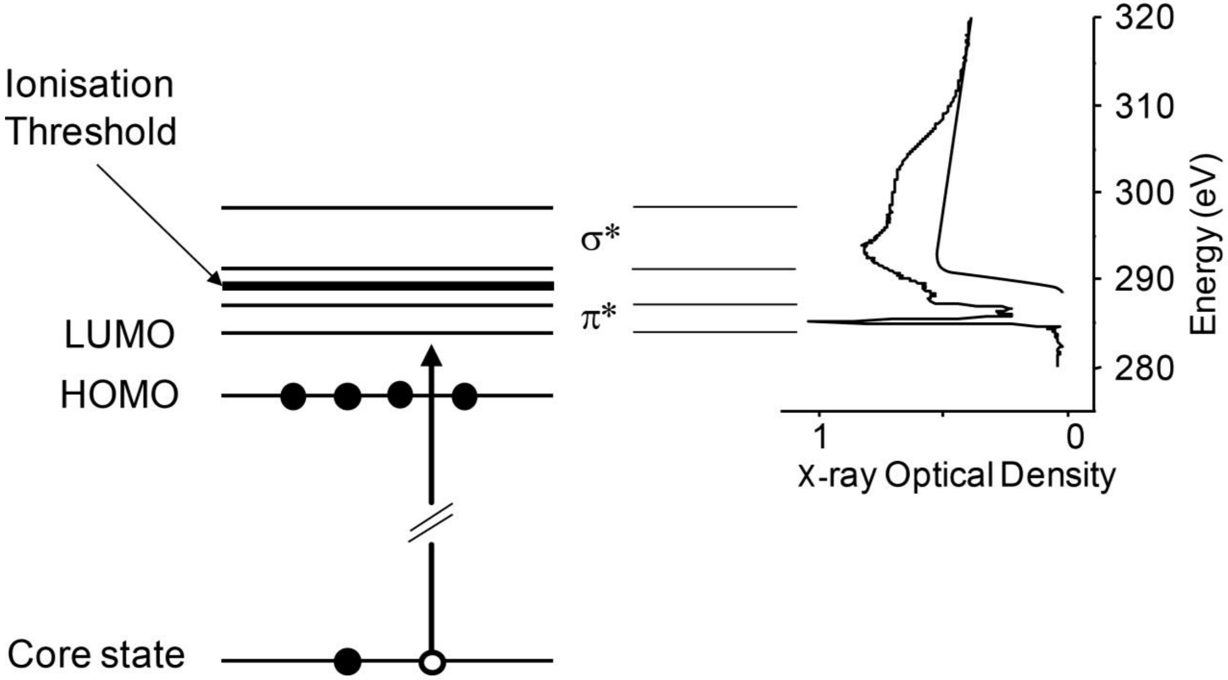


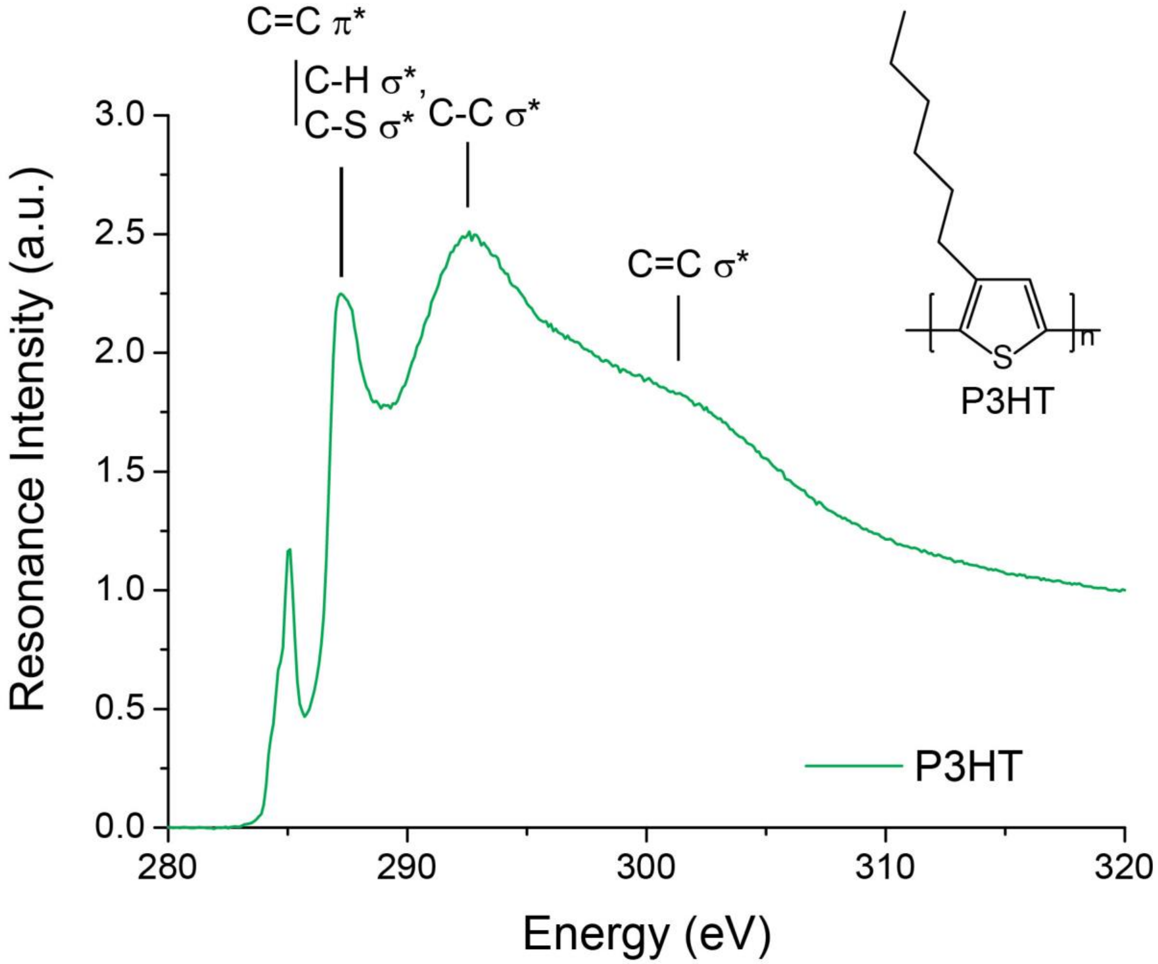
X-rays



https://doi.org/10.1007/978-3-030-64623-3_1

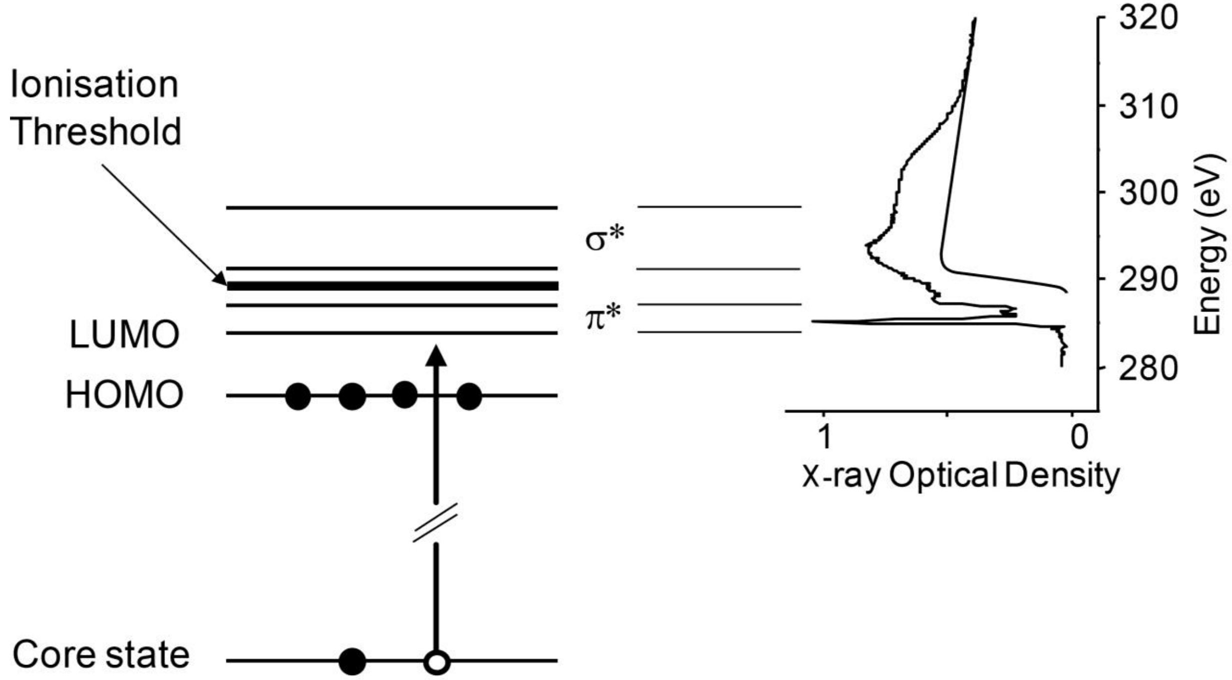
NEXAFS Spectroscopy

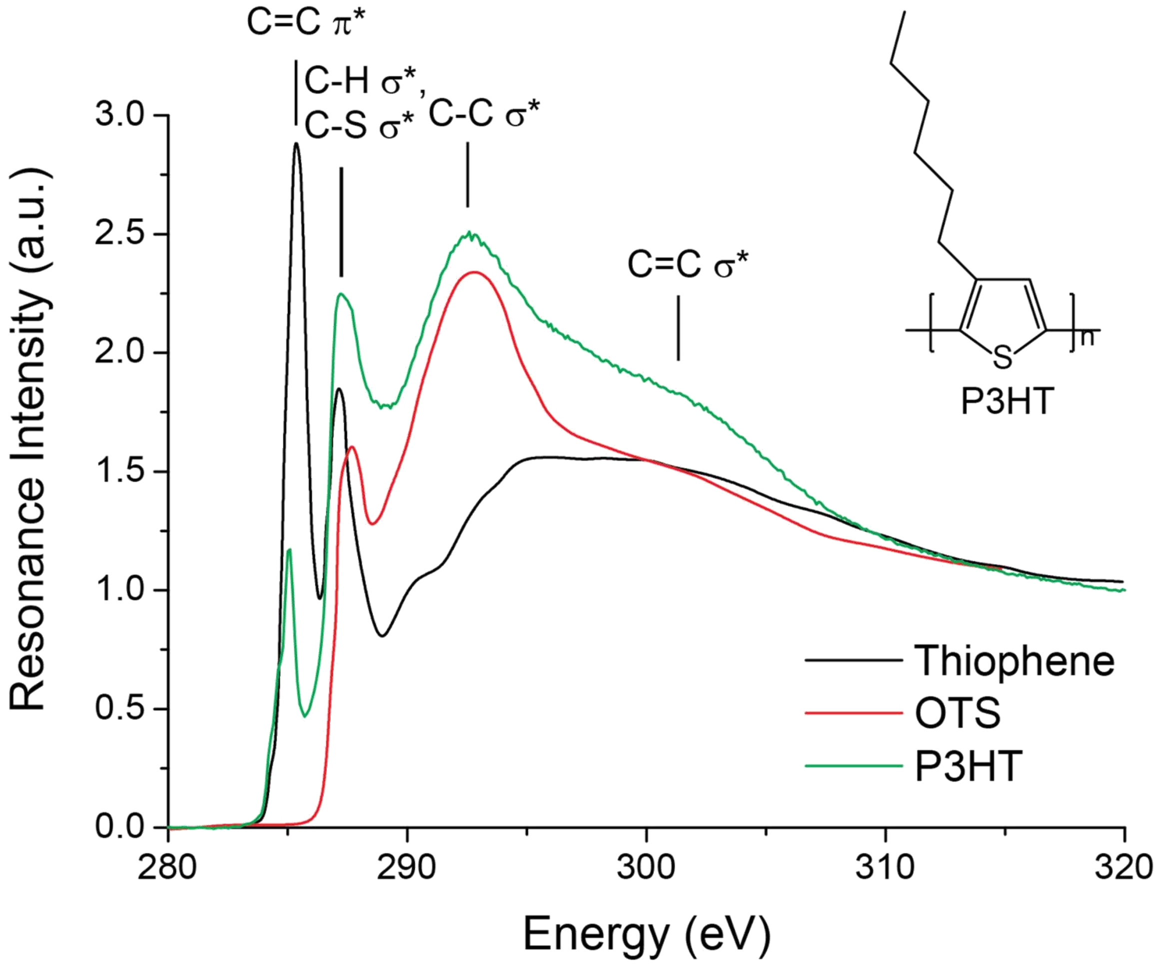




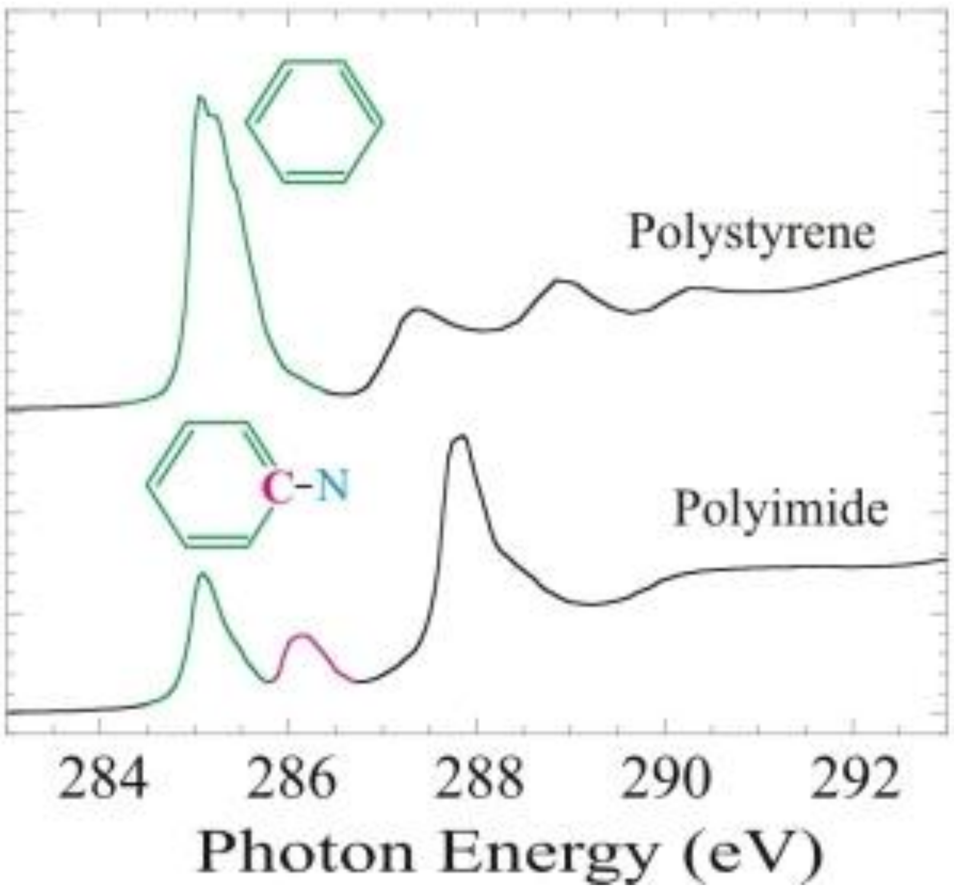
Nahid, Thomsen, and McNeill, *Eur. Polym. J.*, 2016, **81**, 532–554.

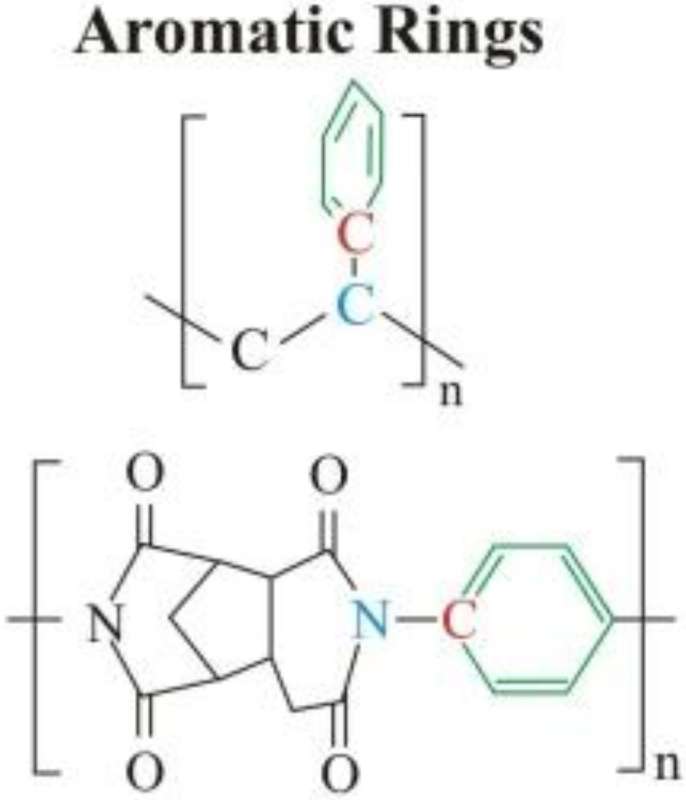
NEXAFS Spectroscopy



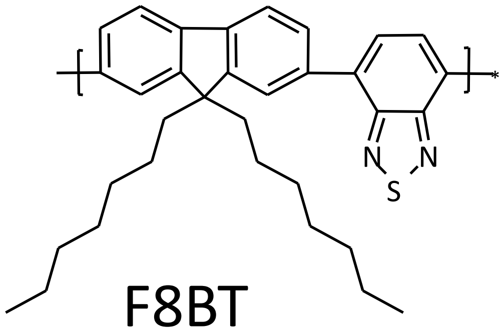


Chemical Fingerprinting

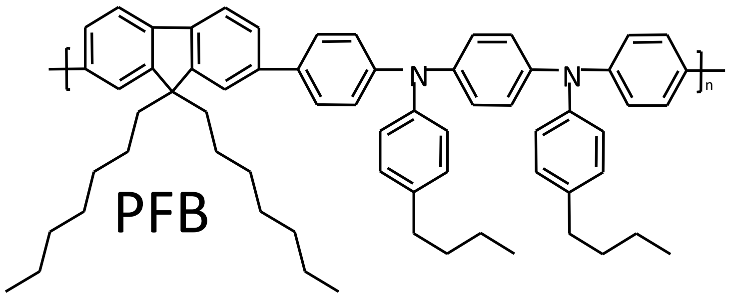




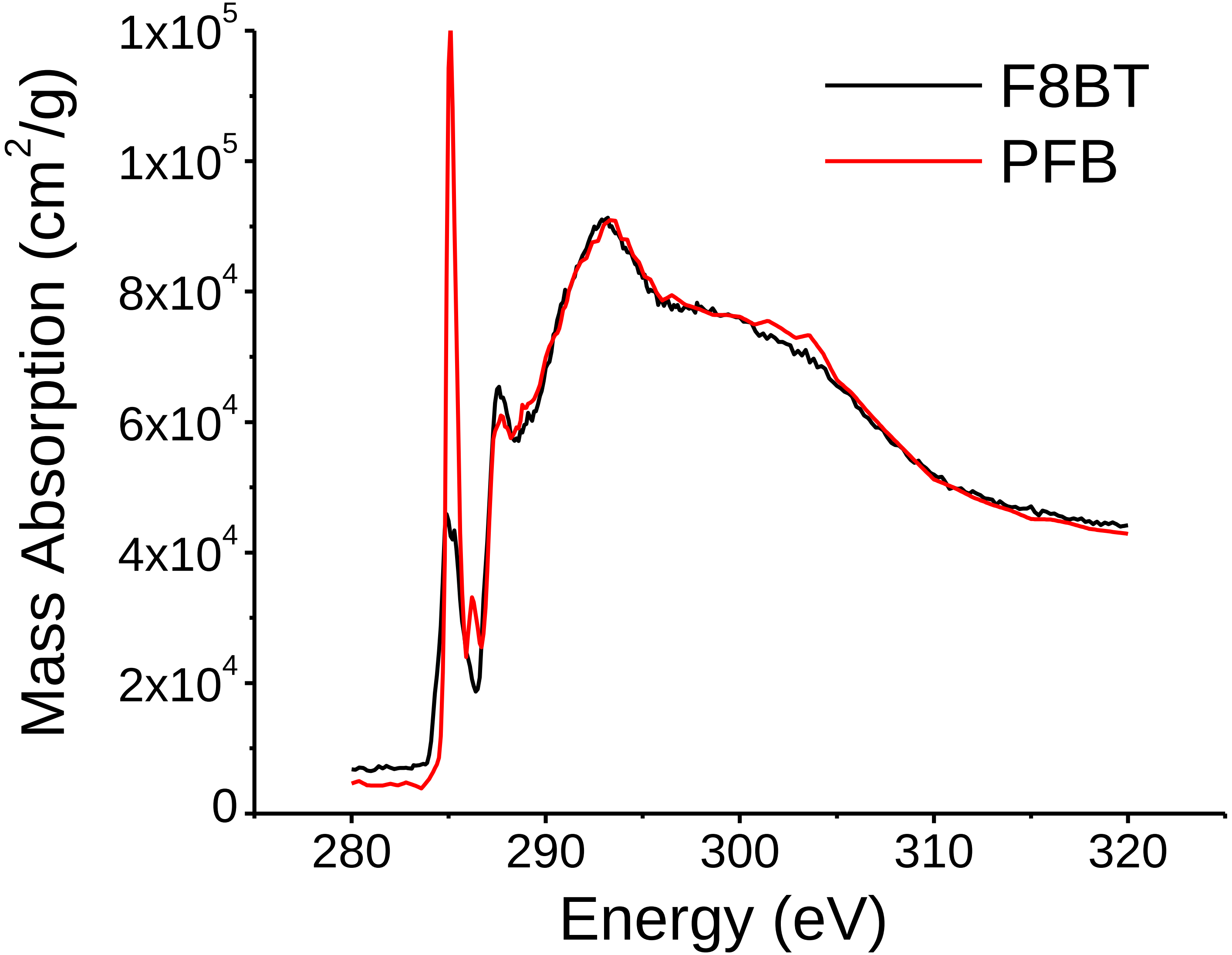
Chemical Contrast



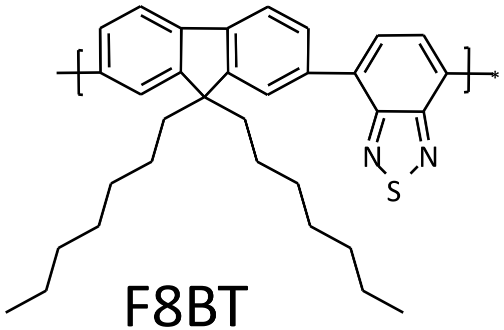
F8BT

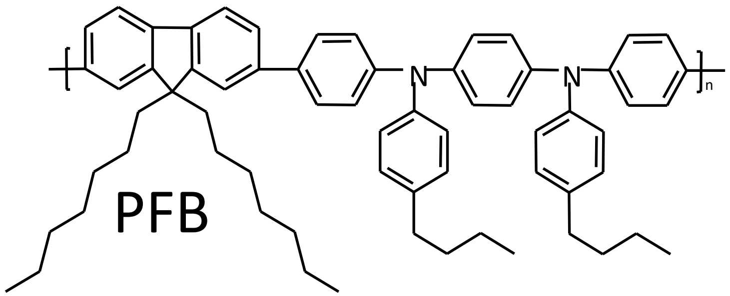


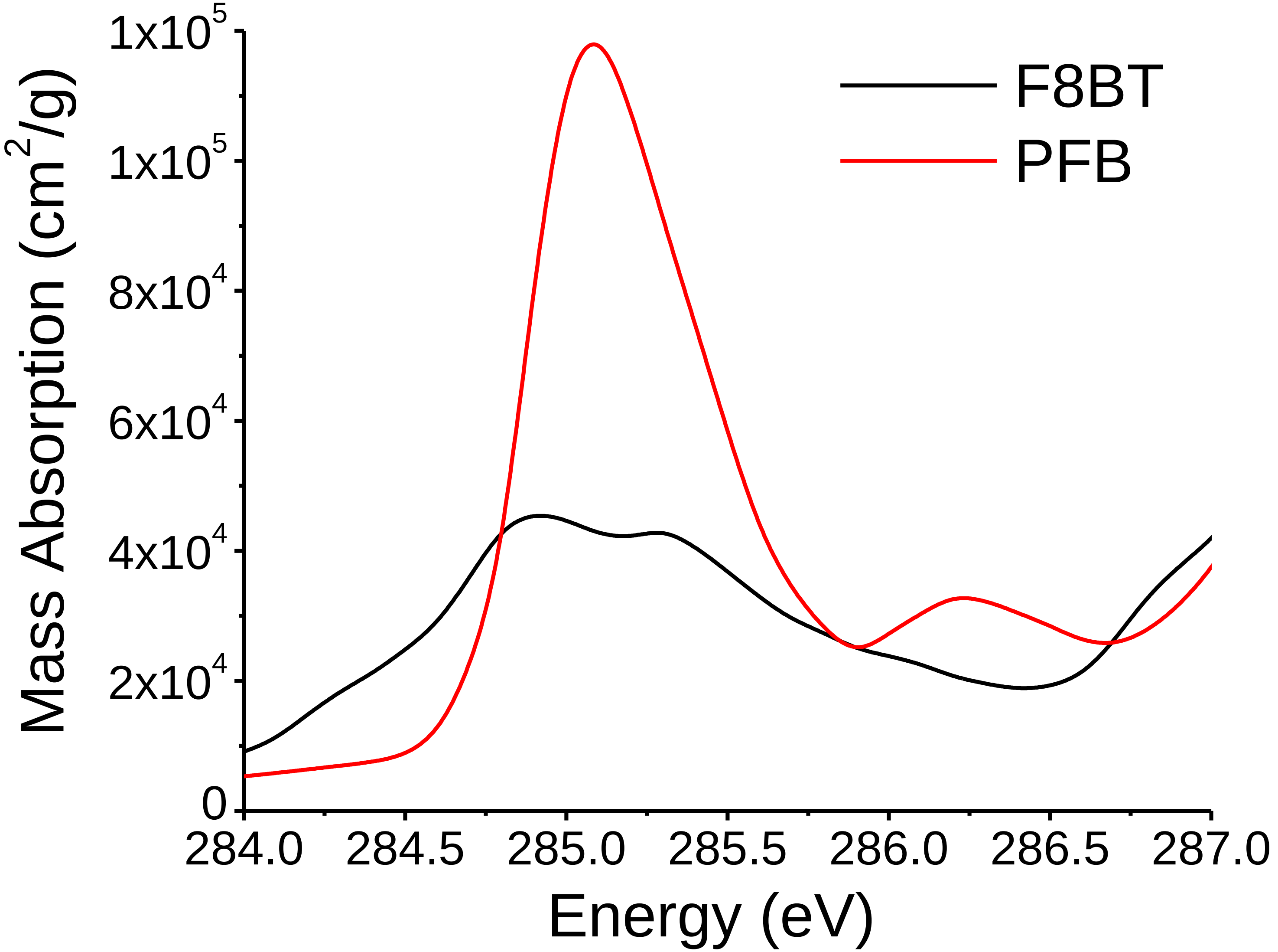
PFB



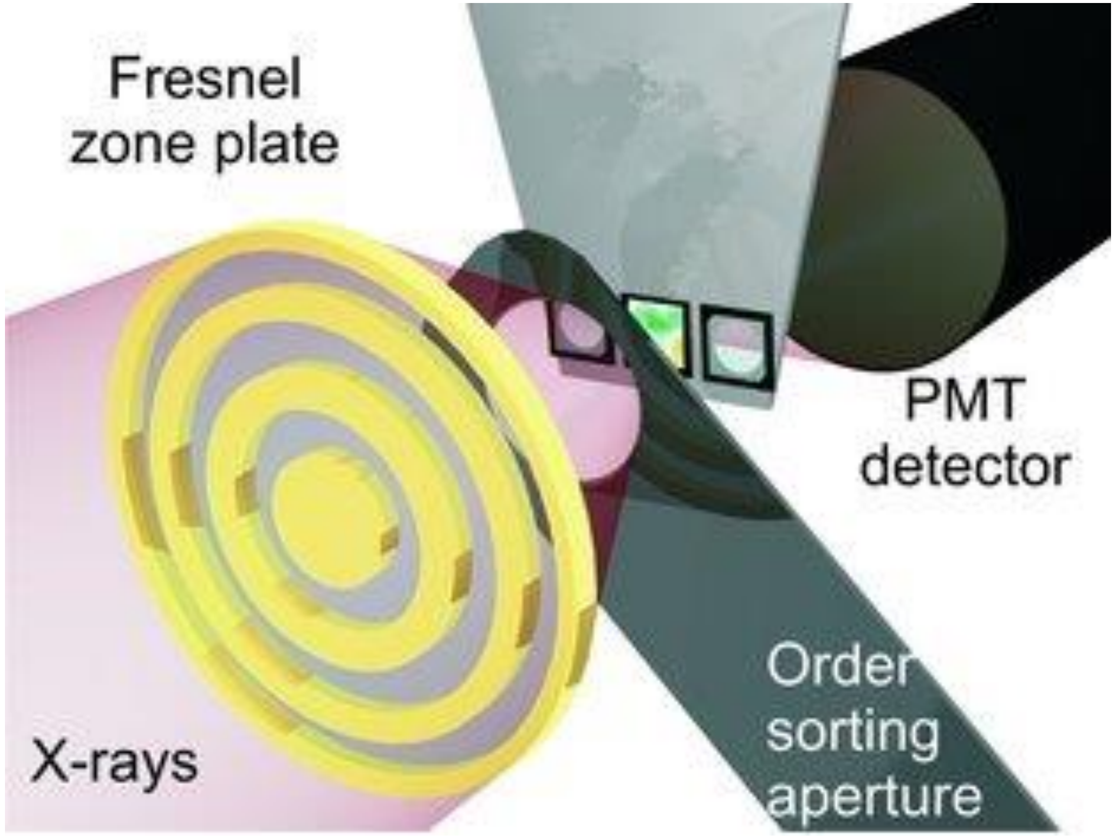
Chemical Contrast

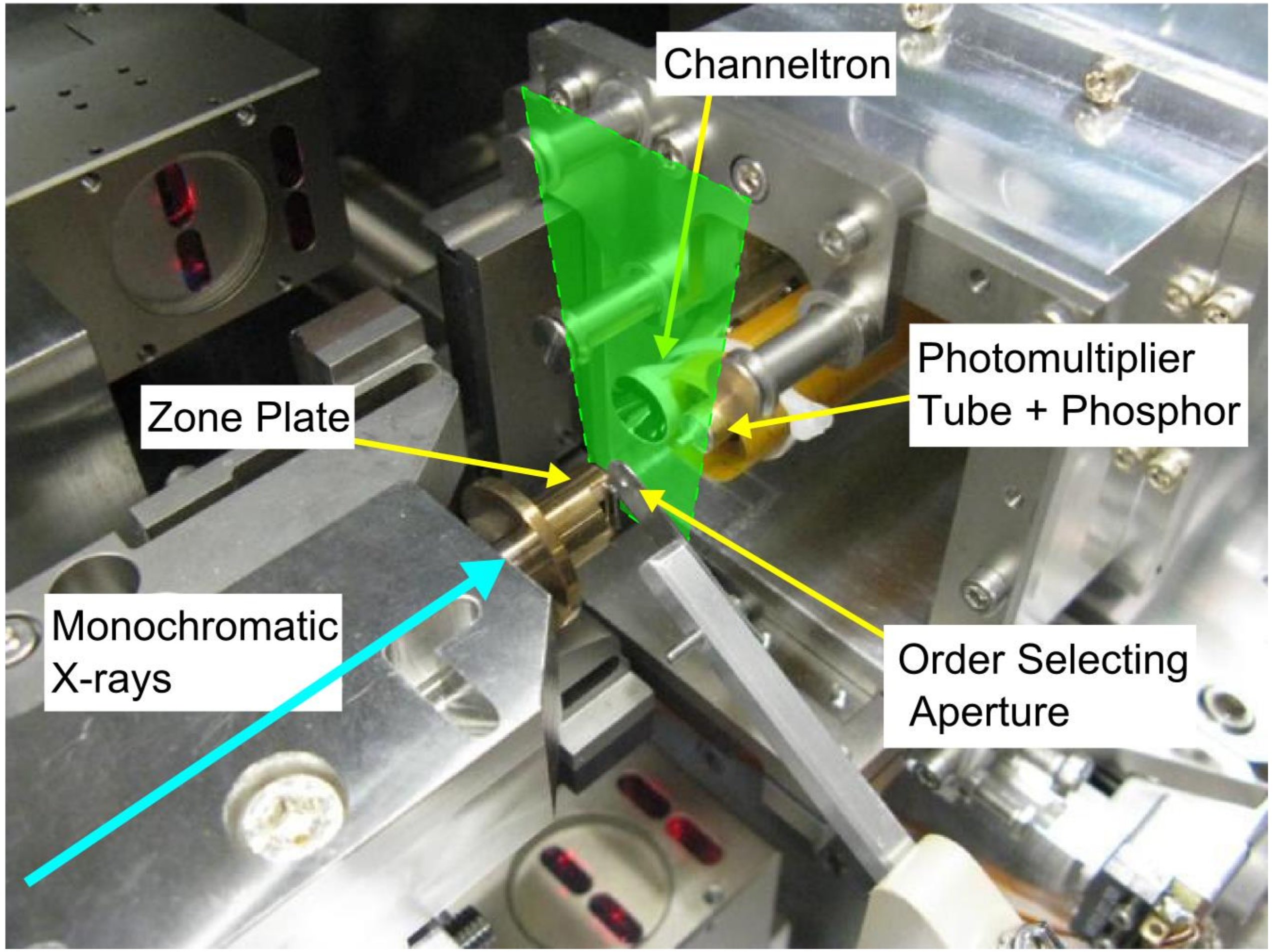




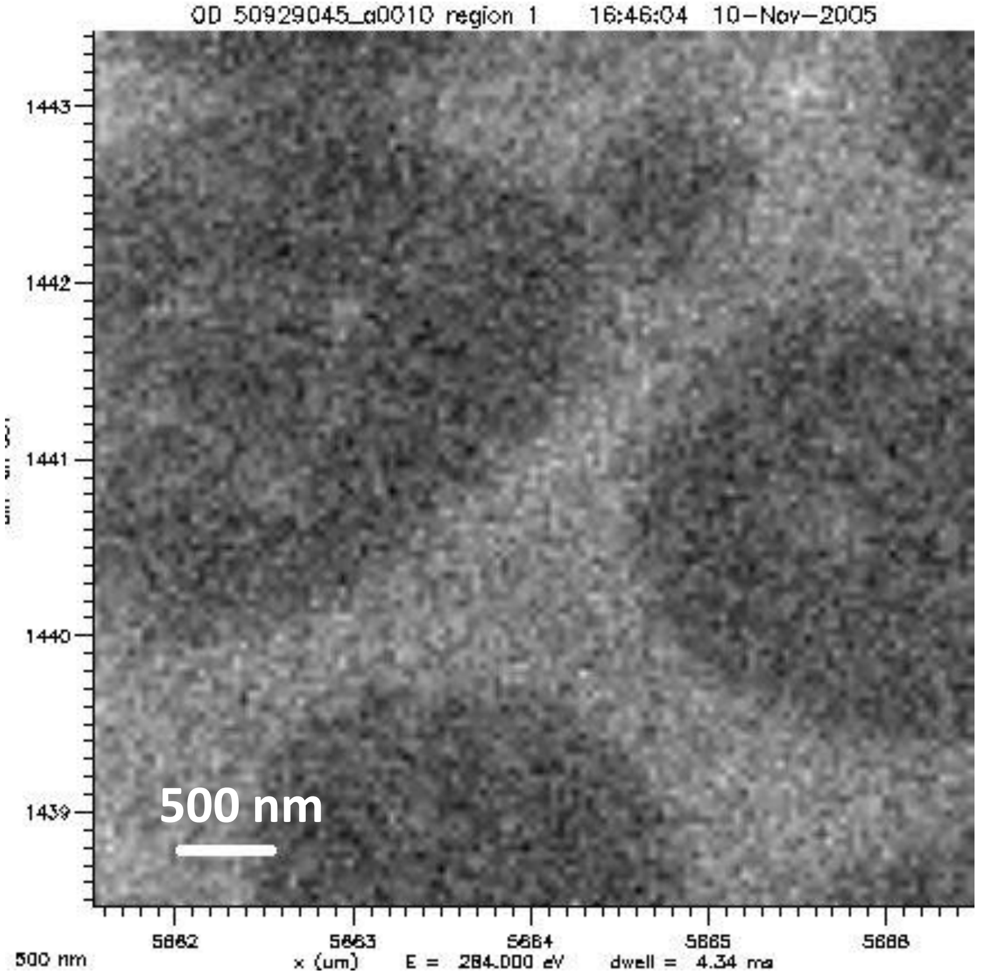


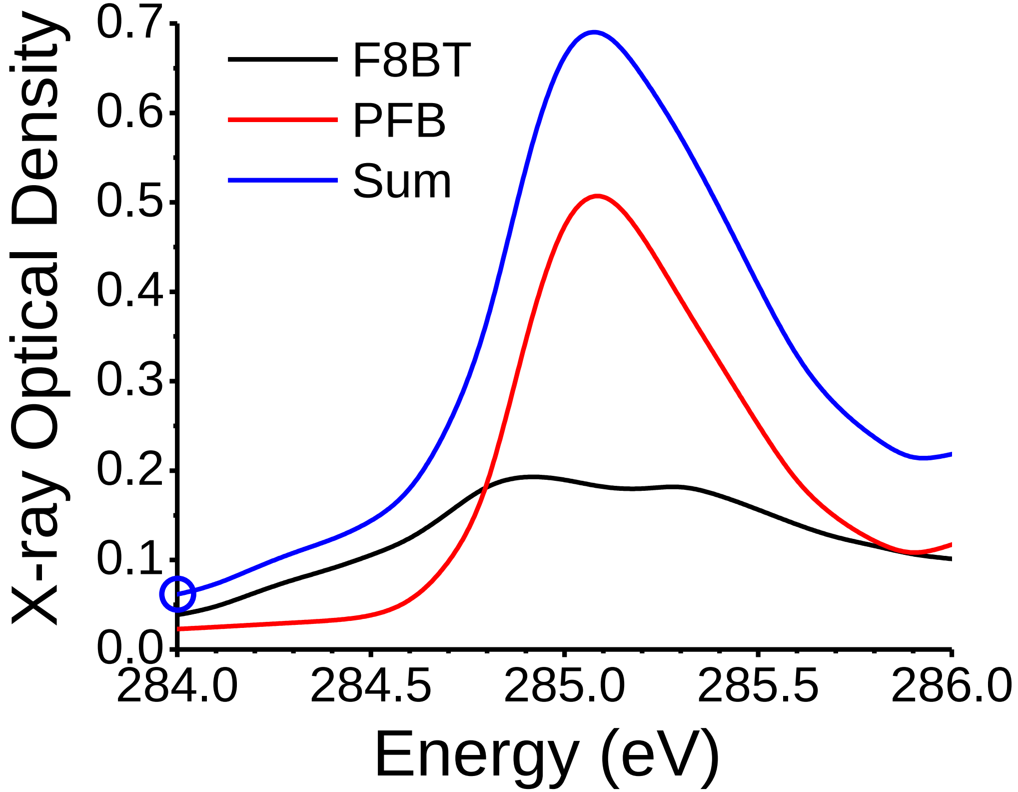
STXM


Fresnel zone plate
PMT detector
X-rays
Order sorting aperture


Channeltron
Photomultiplier Tube + Phosphor
Zone Plate
Monochromatic X-rays
Order Selecting Aperture

STXM of PFB:F8BT Blends

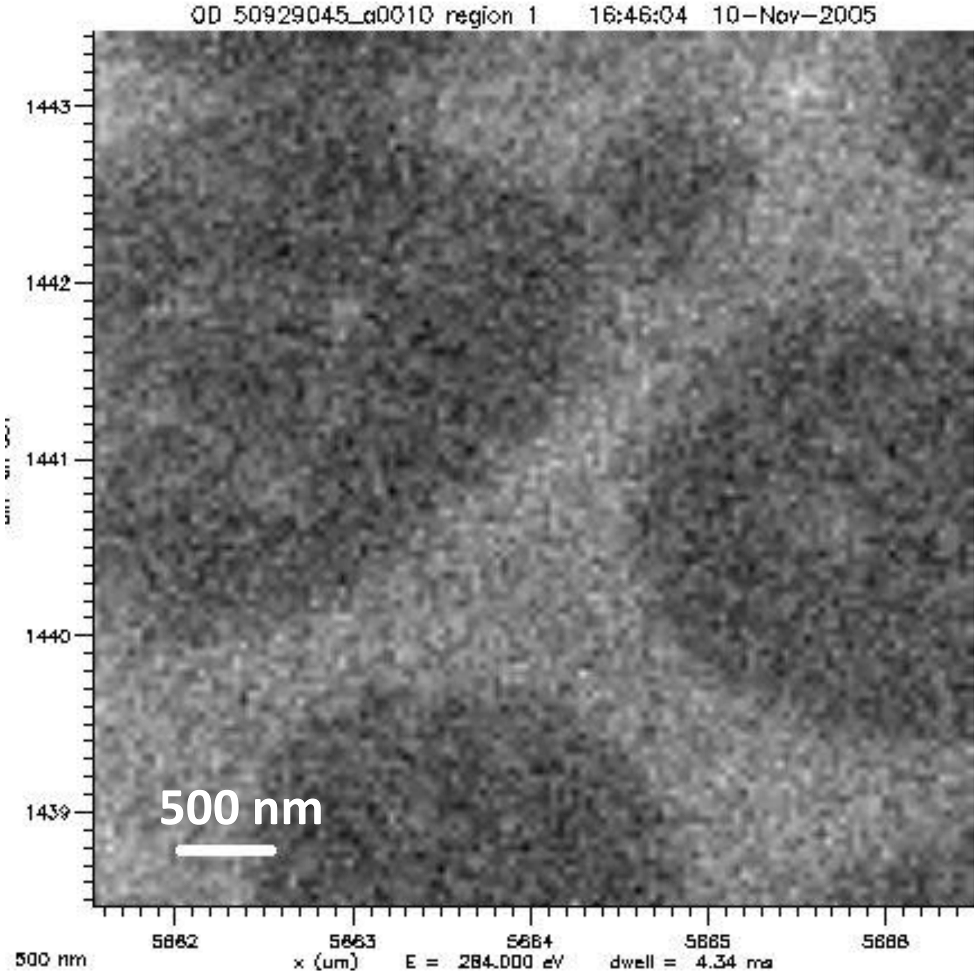


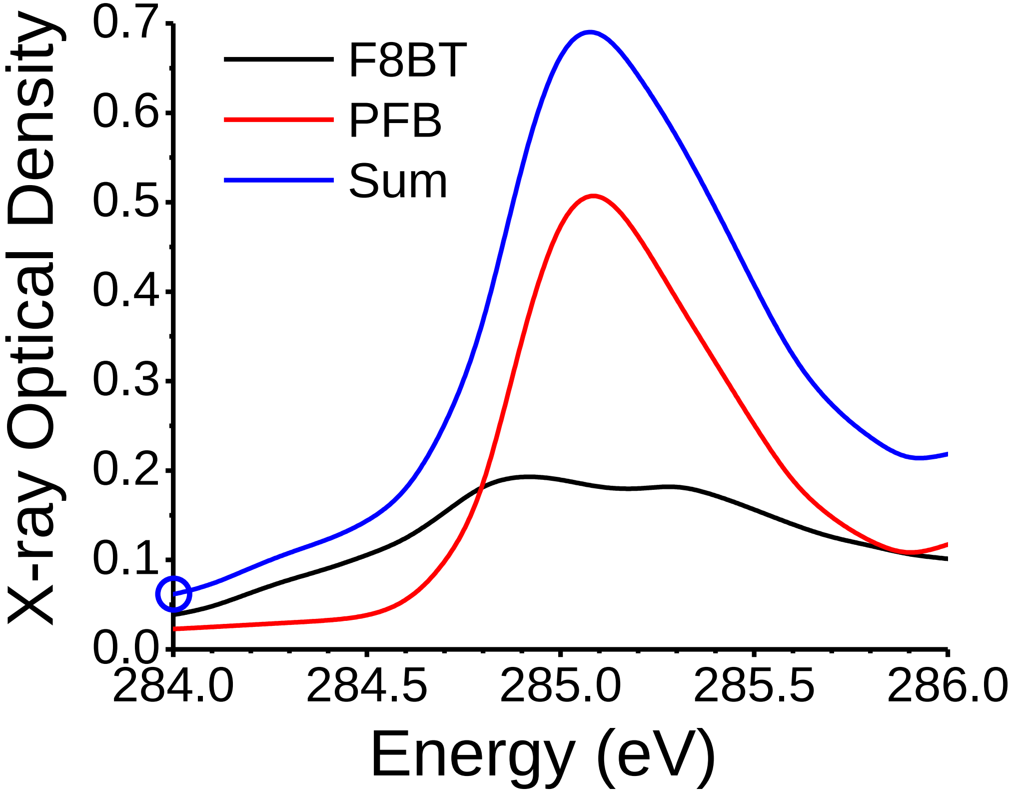


X-ray Energy (eV): 284.0

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

STXM of PFB:F8BT Blends





X-ray Energy (eV): 284.0

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

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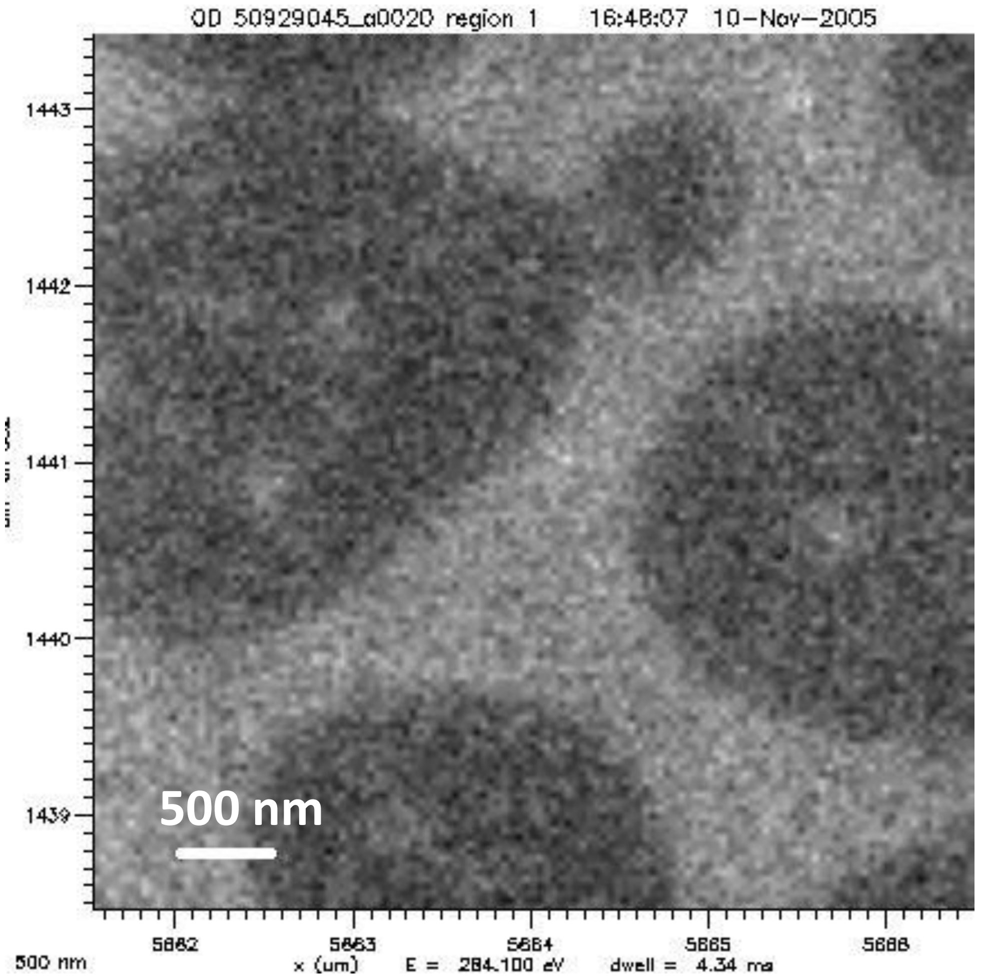
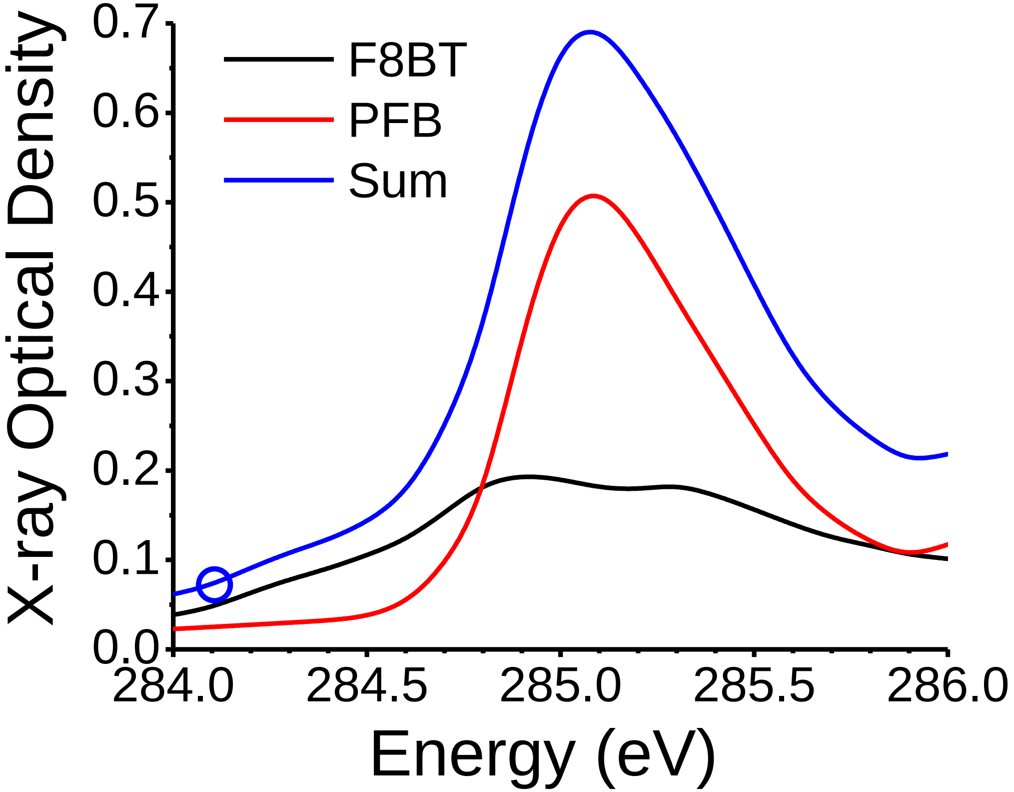
STXM of PFB:F8BT Blends

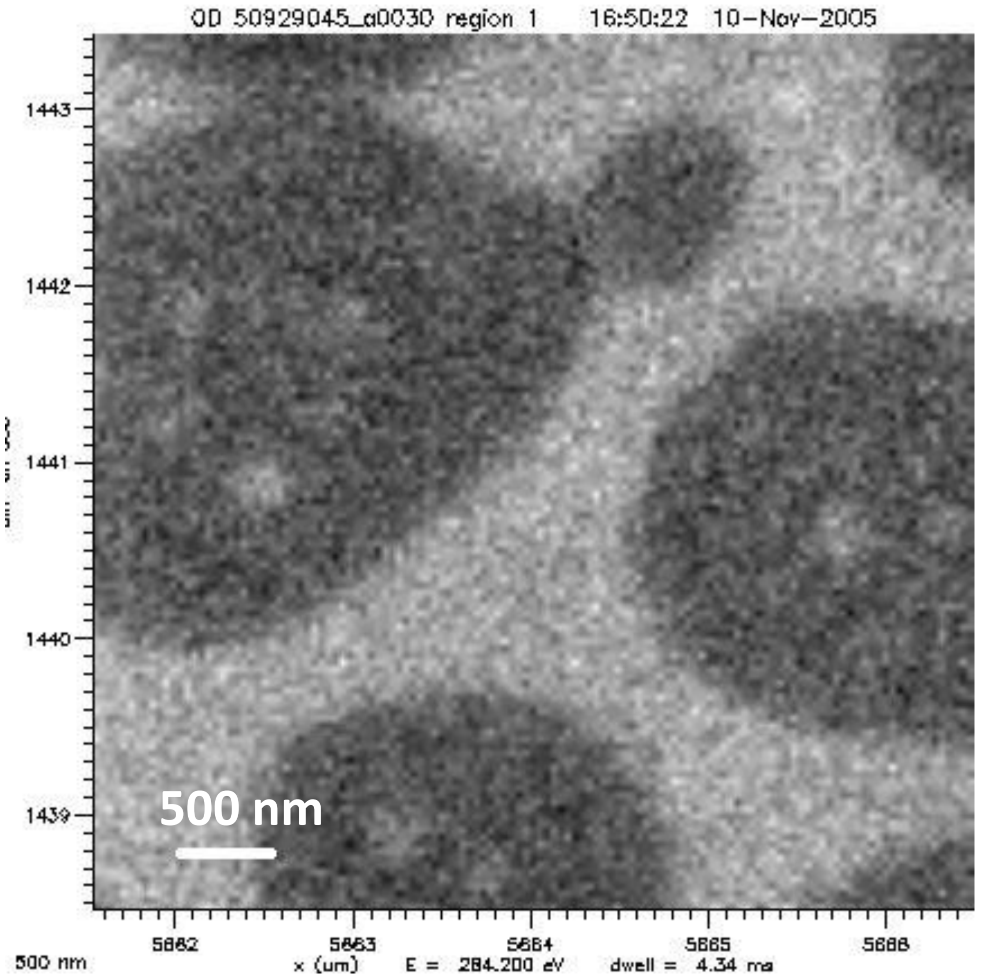


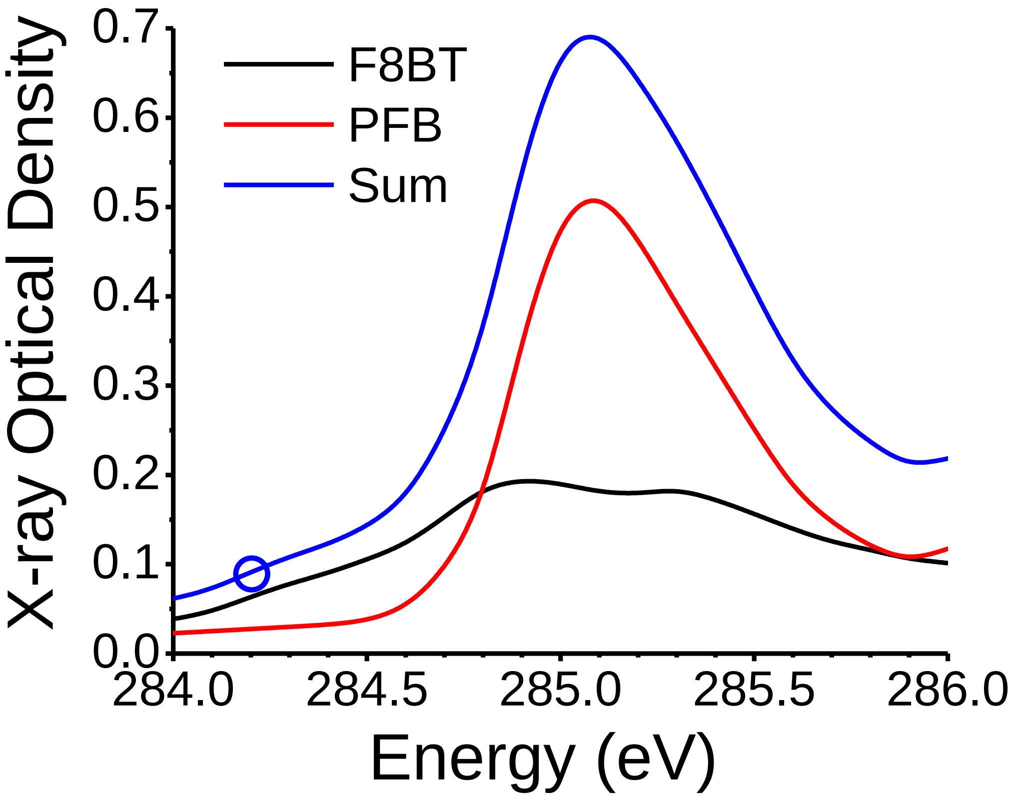


X-ray Energy (eV): 284.1

C. R. McNeill *et al.*, *Nano Lett.* **6**, 1202 (2006).

STXM of PFB:F8BT Blends

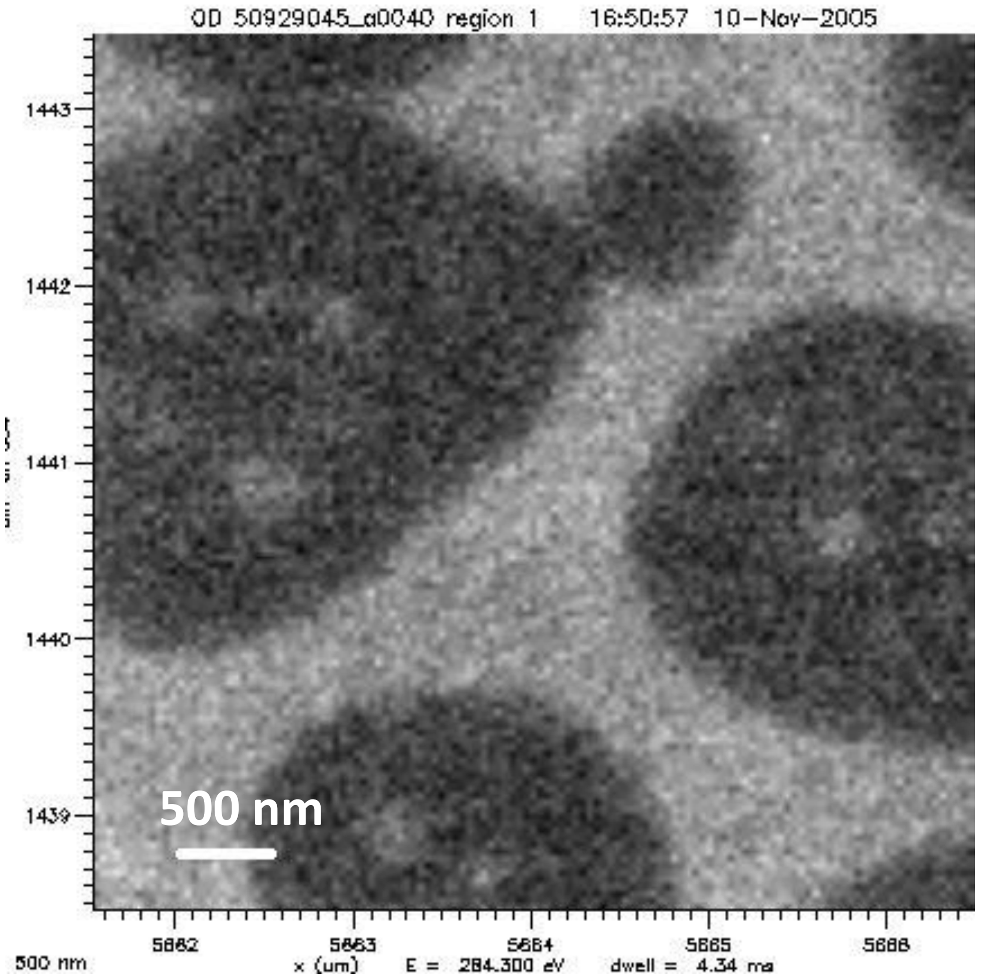


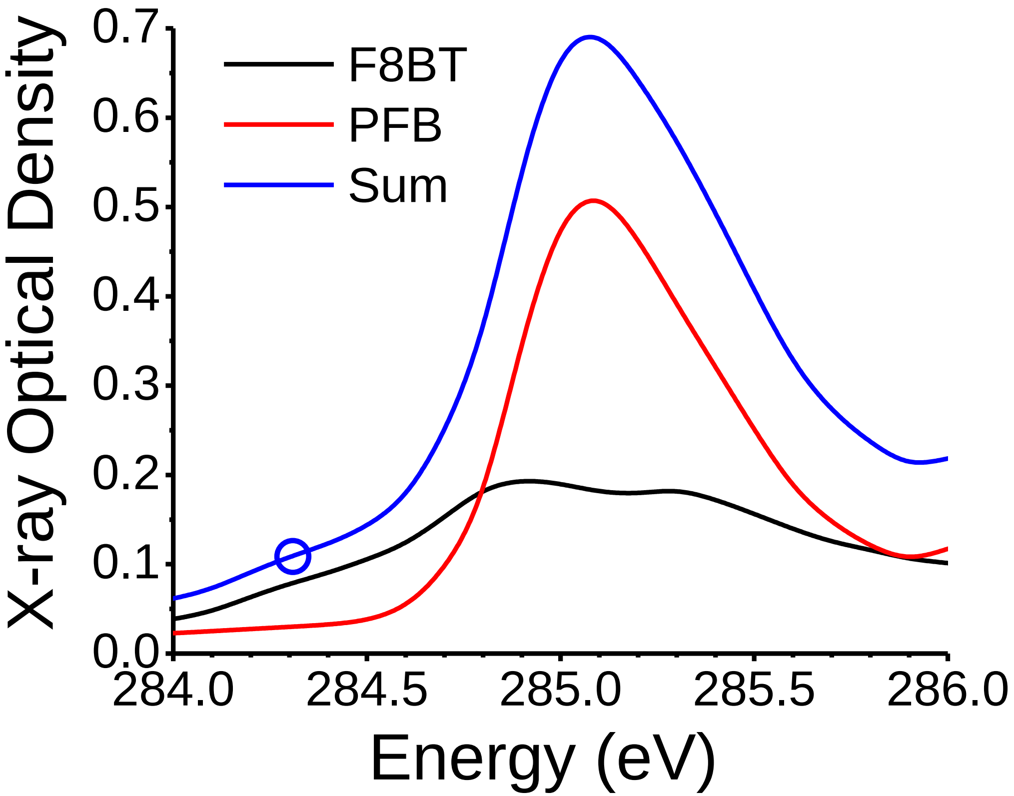


X-ray Energy (eV): 284.2

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

STXM of PFB:F8BT Blends

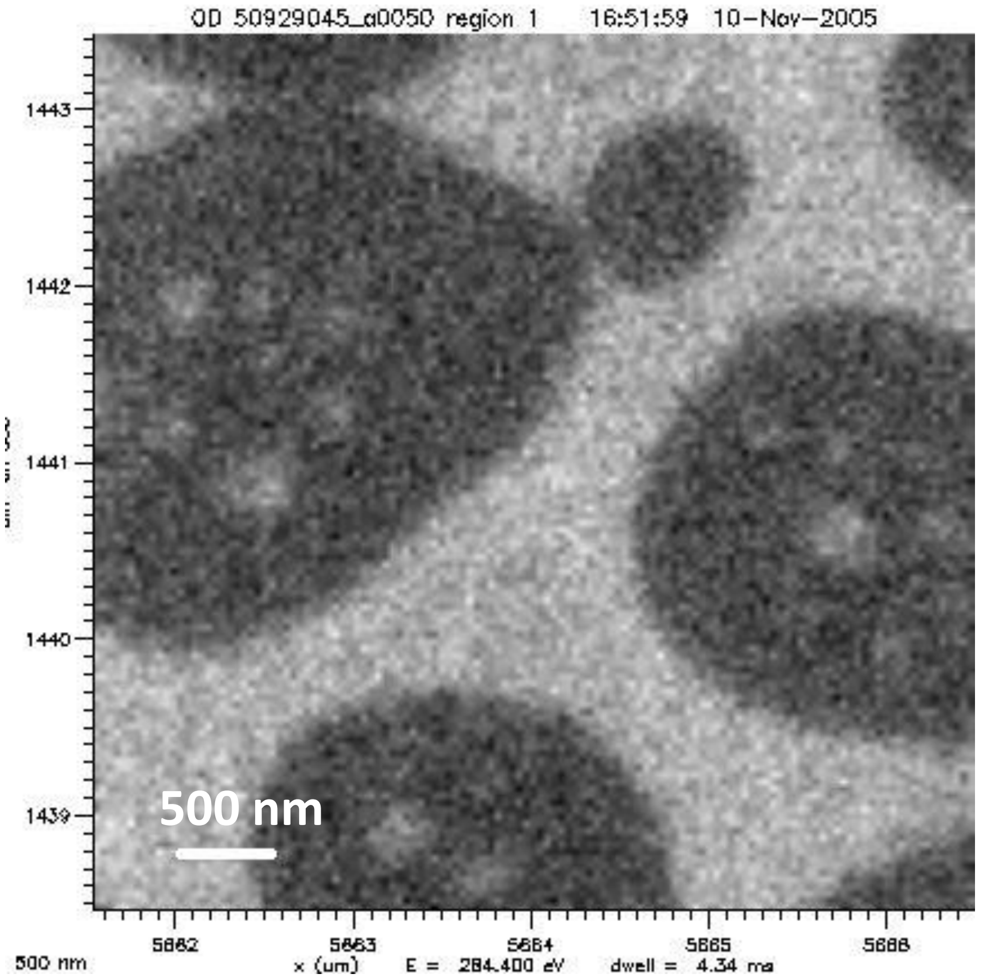


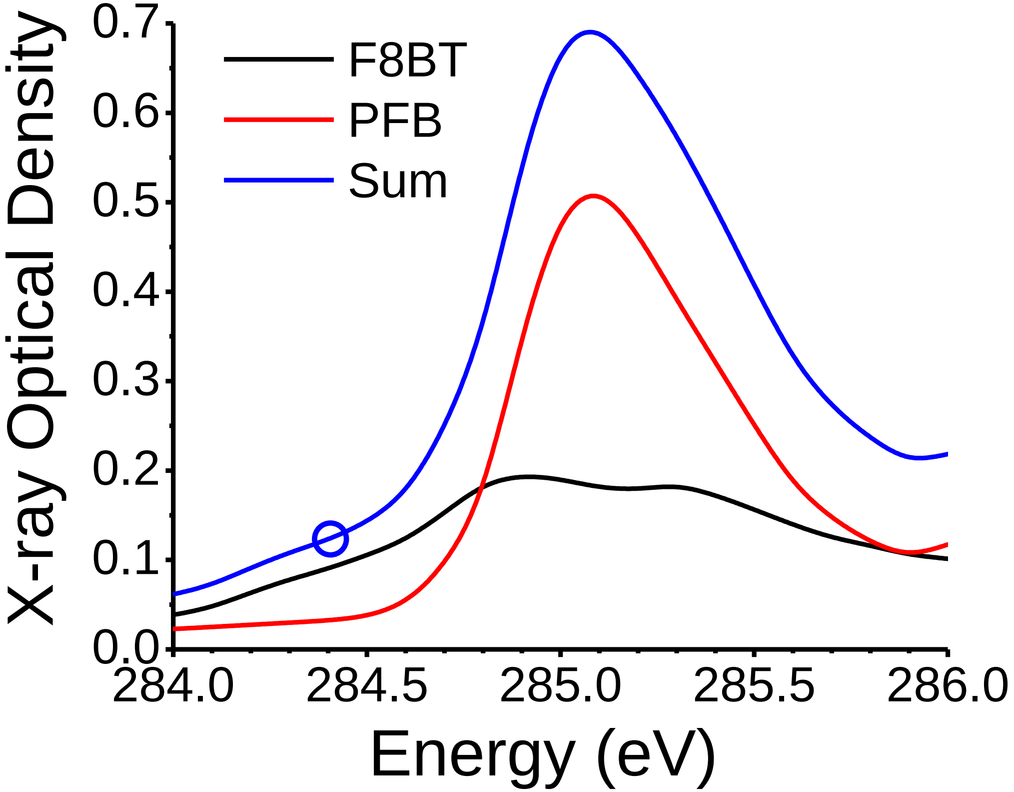


X-ray Energy (eV): 284.3

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

STXM of PFB:F8BT Blends

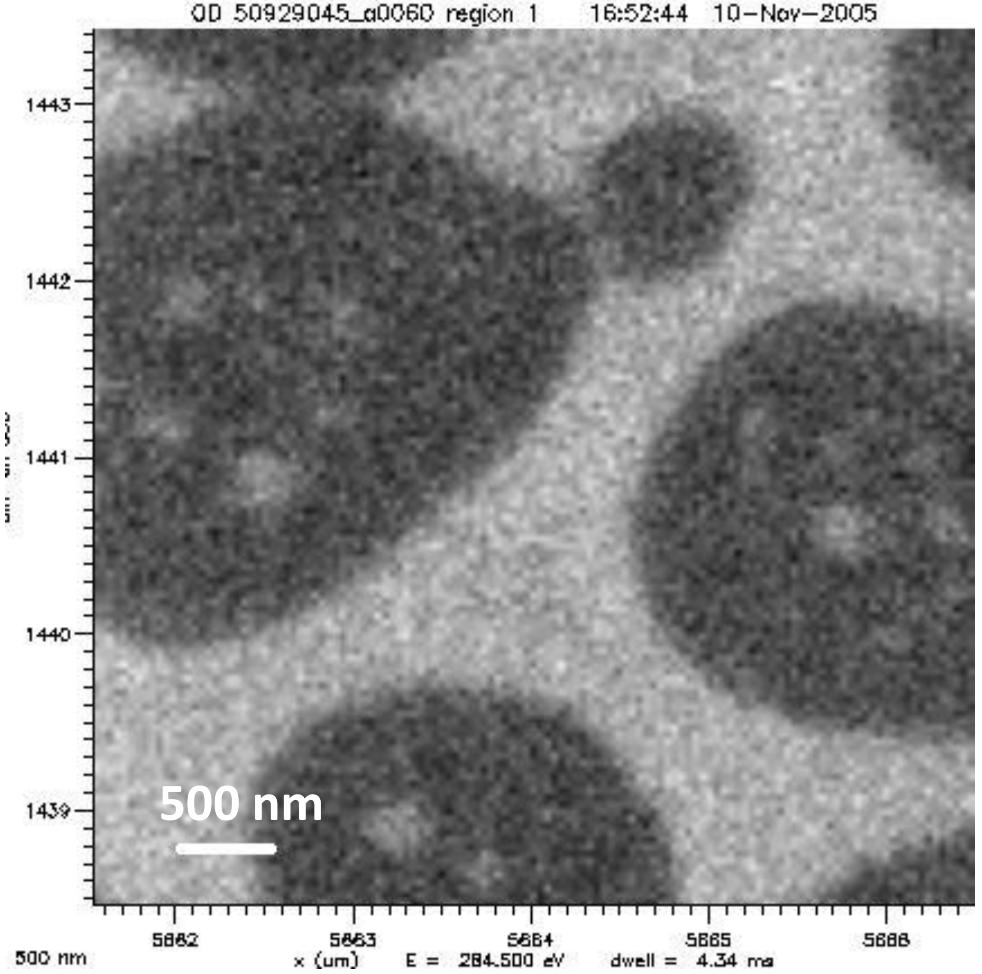


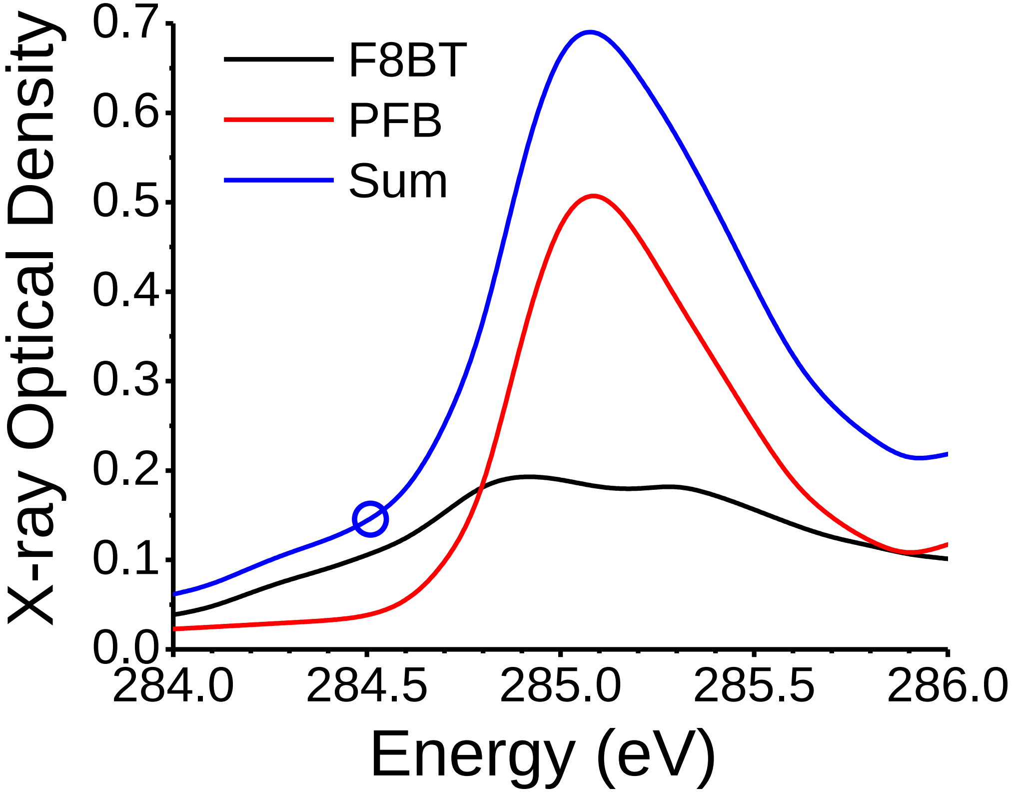


X-ray Energy (eV): 284.4

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

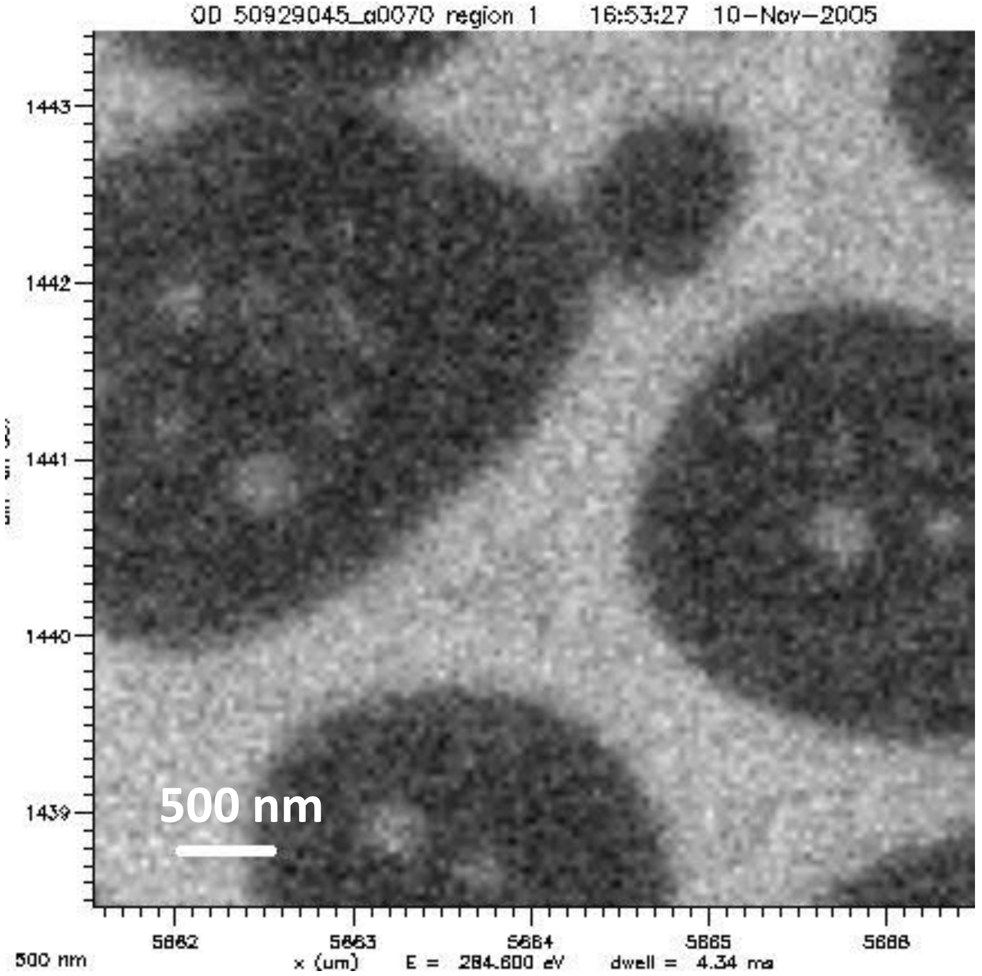
STXM of PFB:F8BT Blends

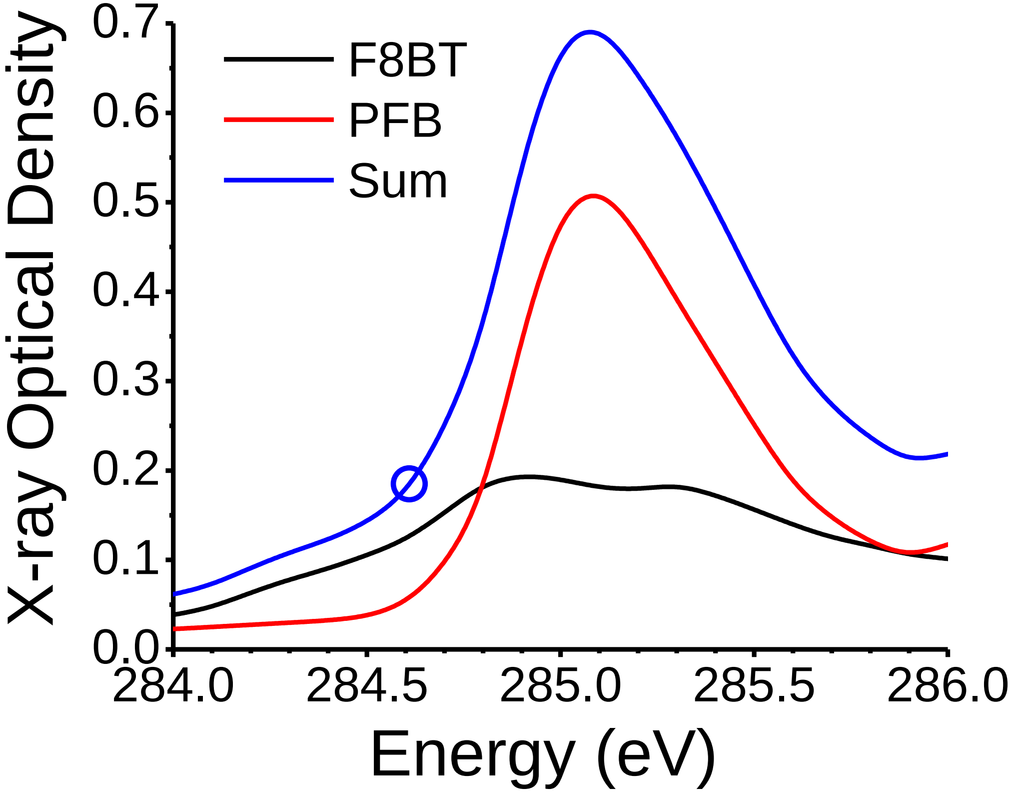




X-ray Energy (eV): 284.5

STXM of PFB:F8BT Blends





X-ray Energy (eV): 284.6

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

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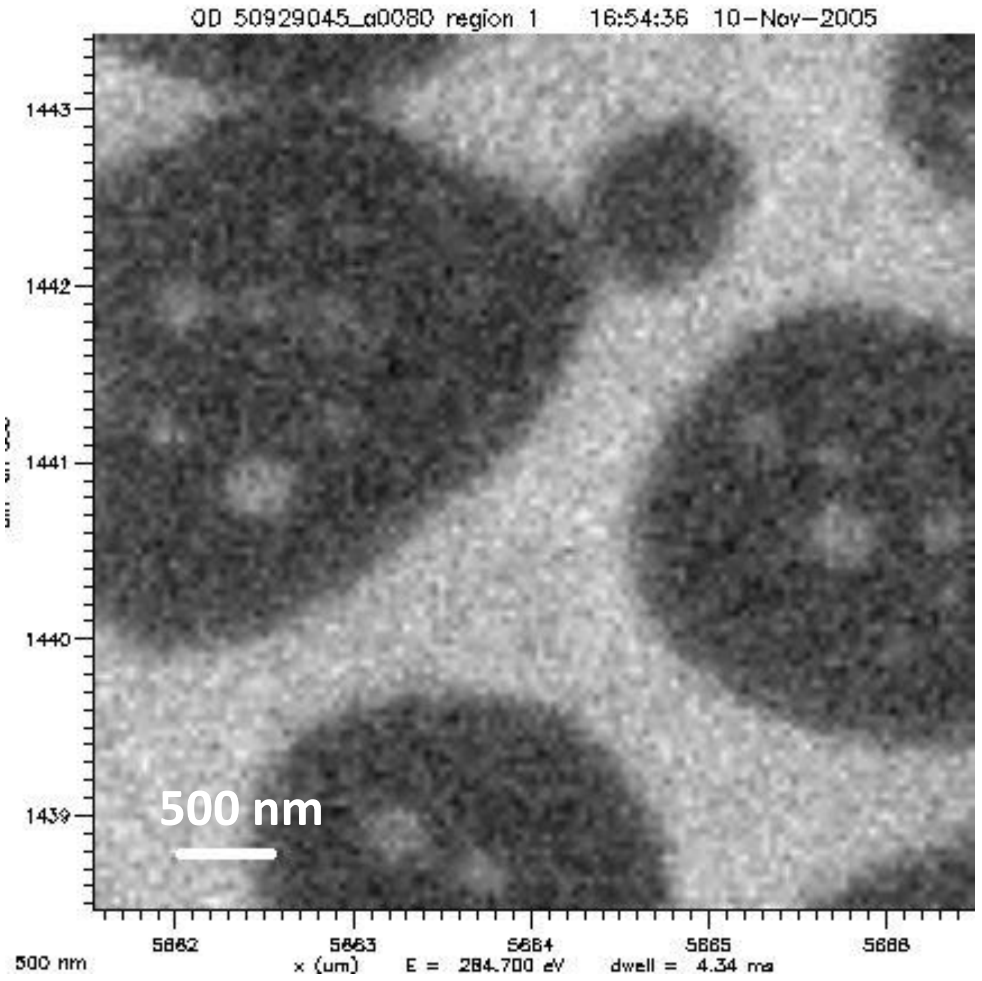
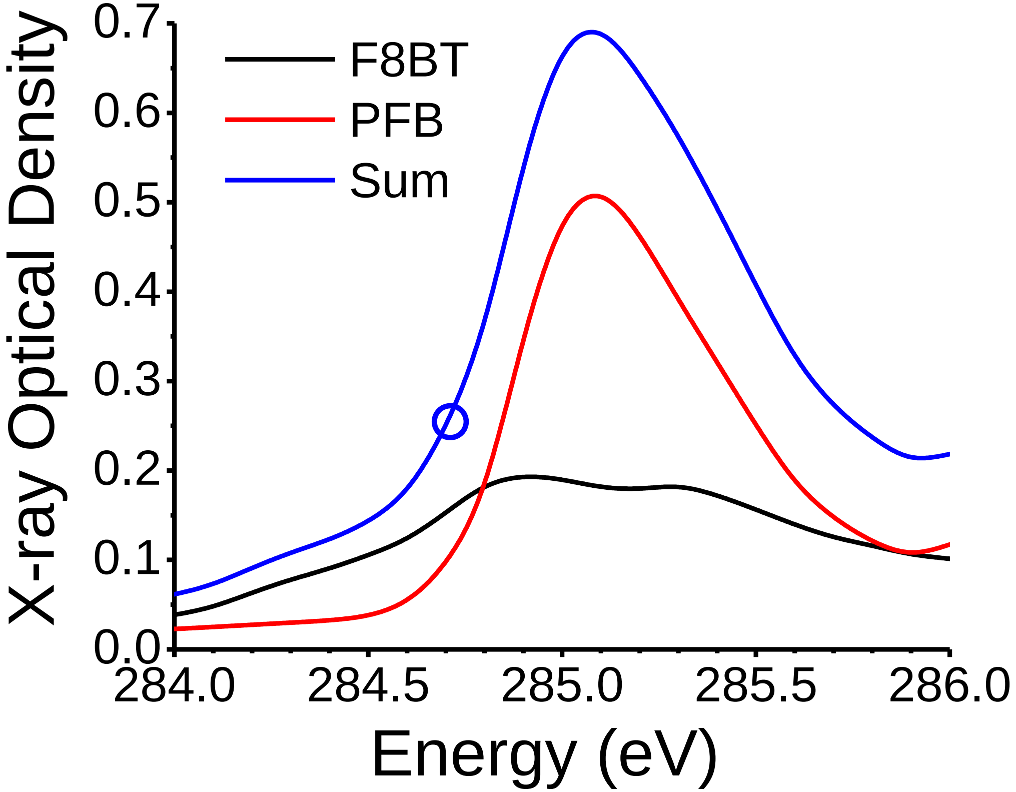
STXM of PFB:F8BT Blends

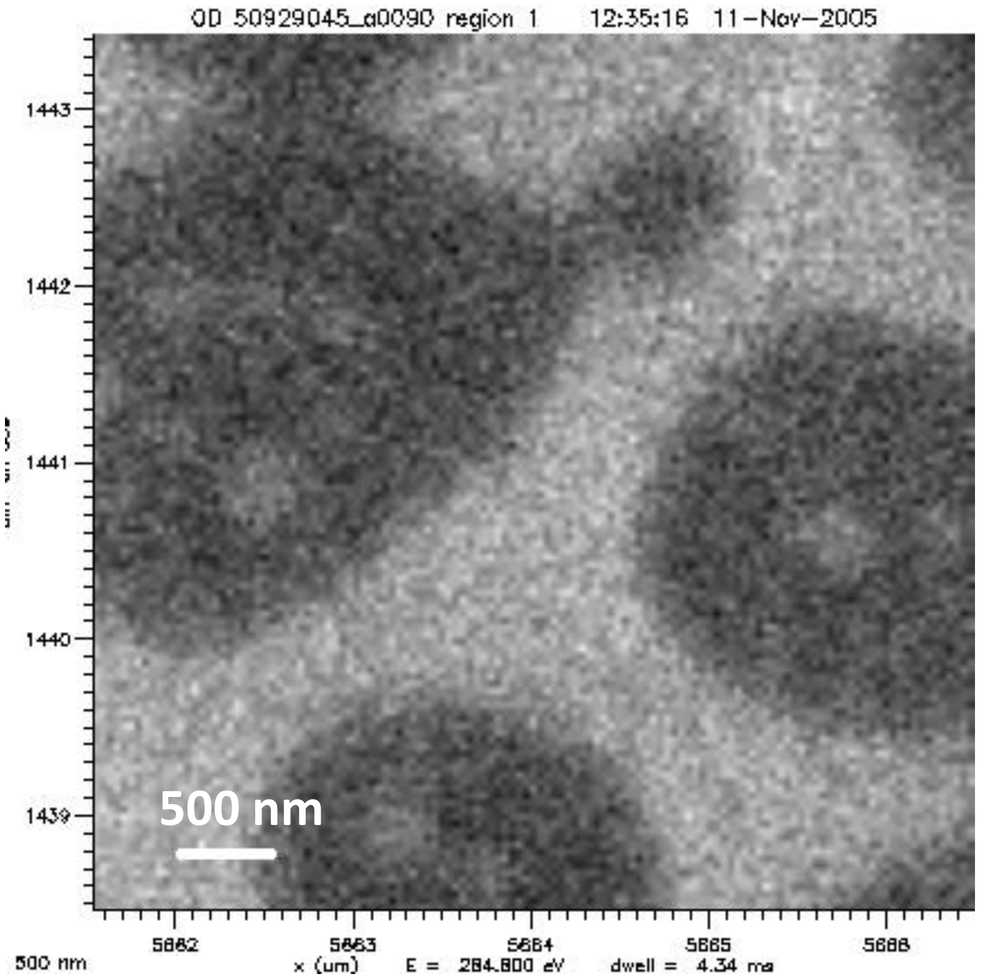


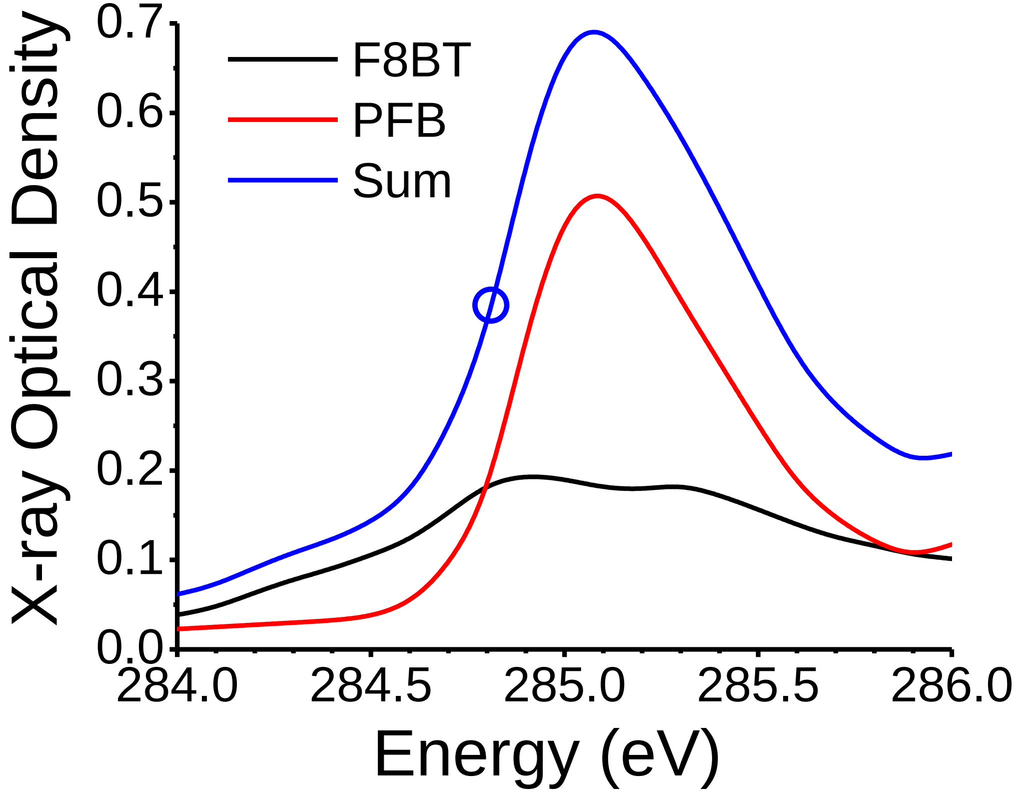


X-ray Energy (eV): 284.7

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

STXM of PFB:F8BT Blends





X-ray Energy (eV): 284.8

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

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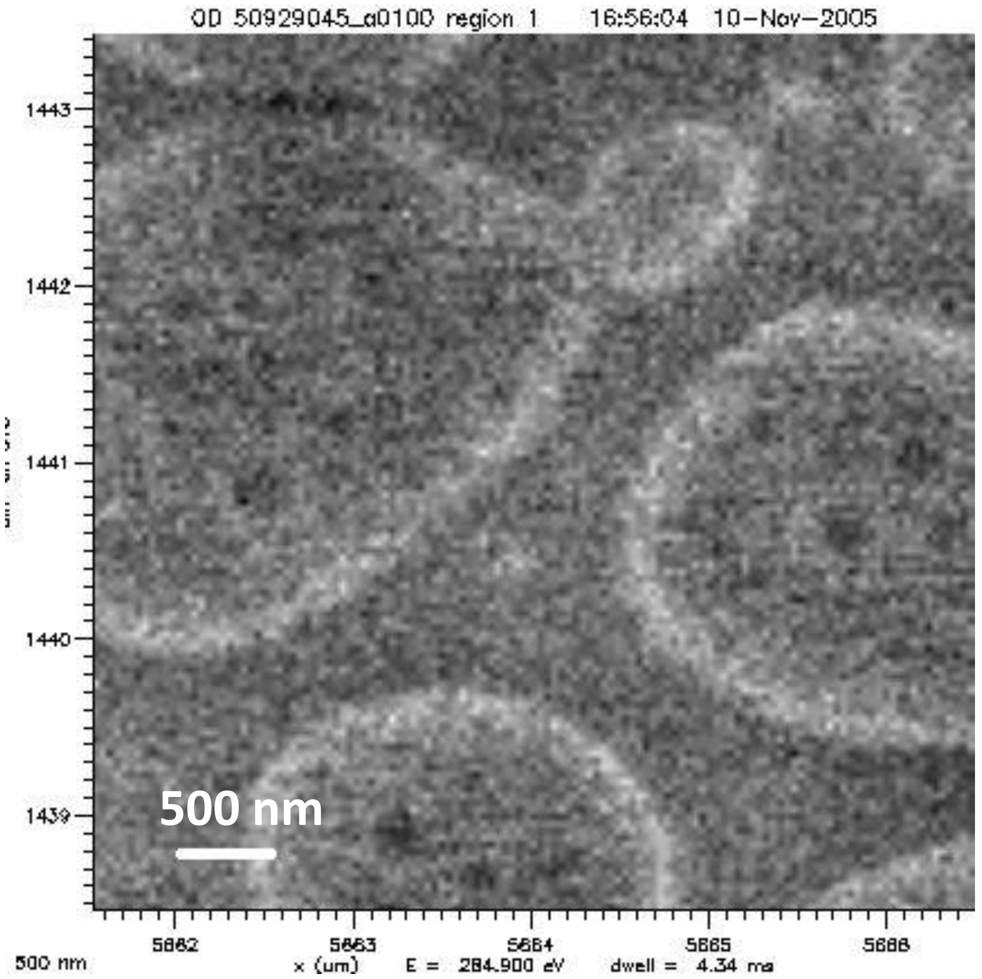
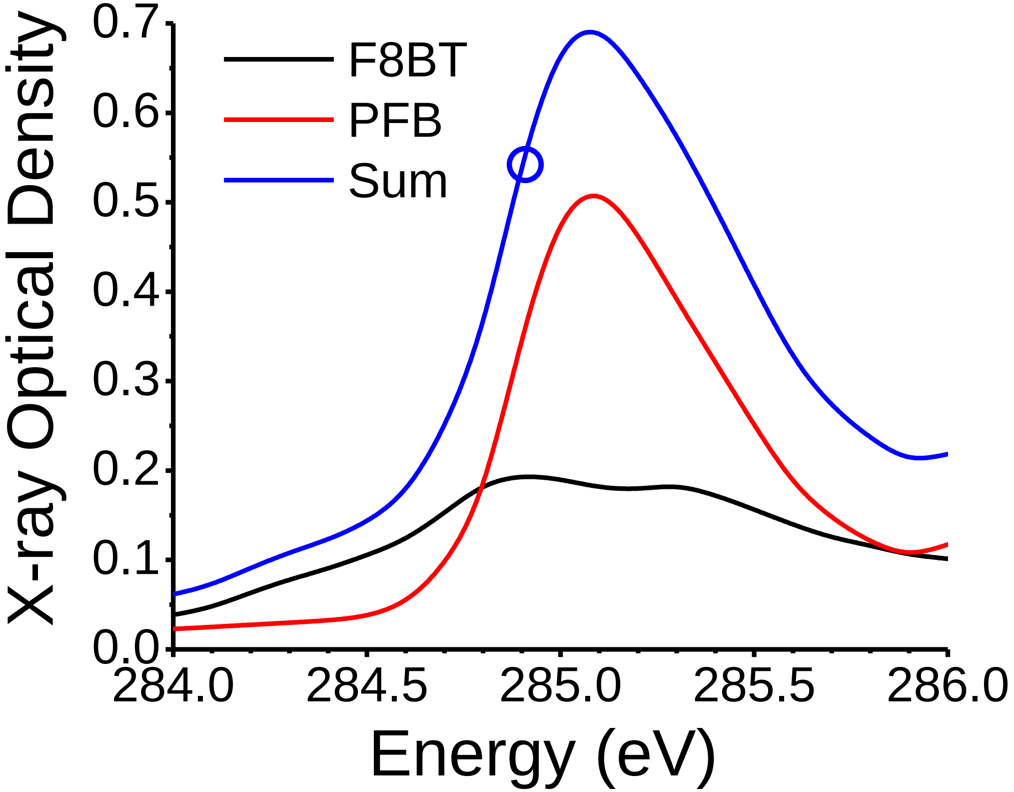
STXM of PFB:F8BT Blends





X-ray Energy (eV): 284.9

C. R. McNeill *et al.*, *Nano Lett.* **6**, 1202 (2006).

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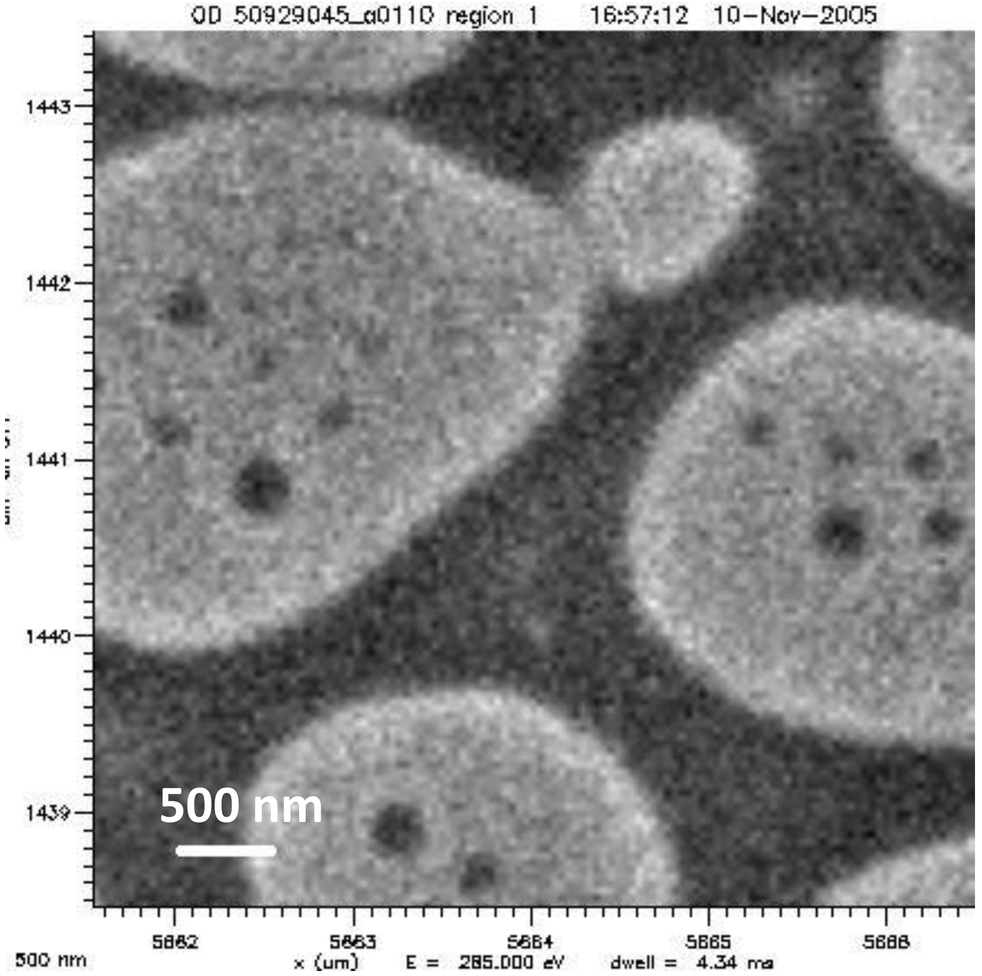
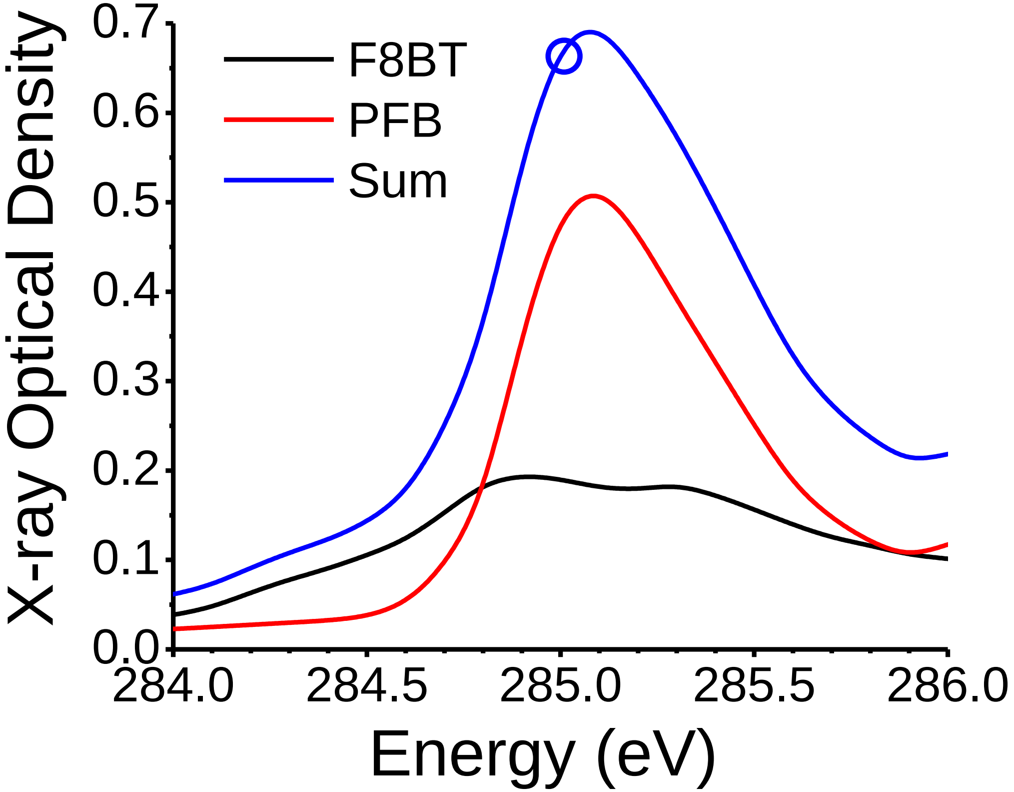
STXM of PFB:F8BT Blends





X-ray Energy (eV): 285.0

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

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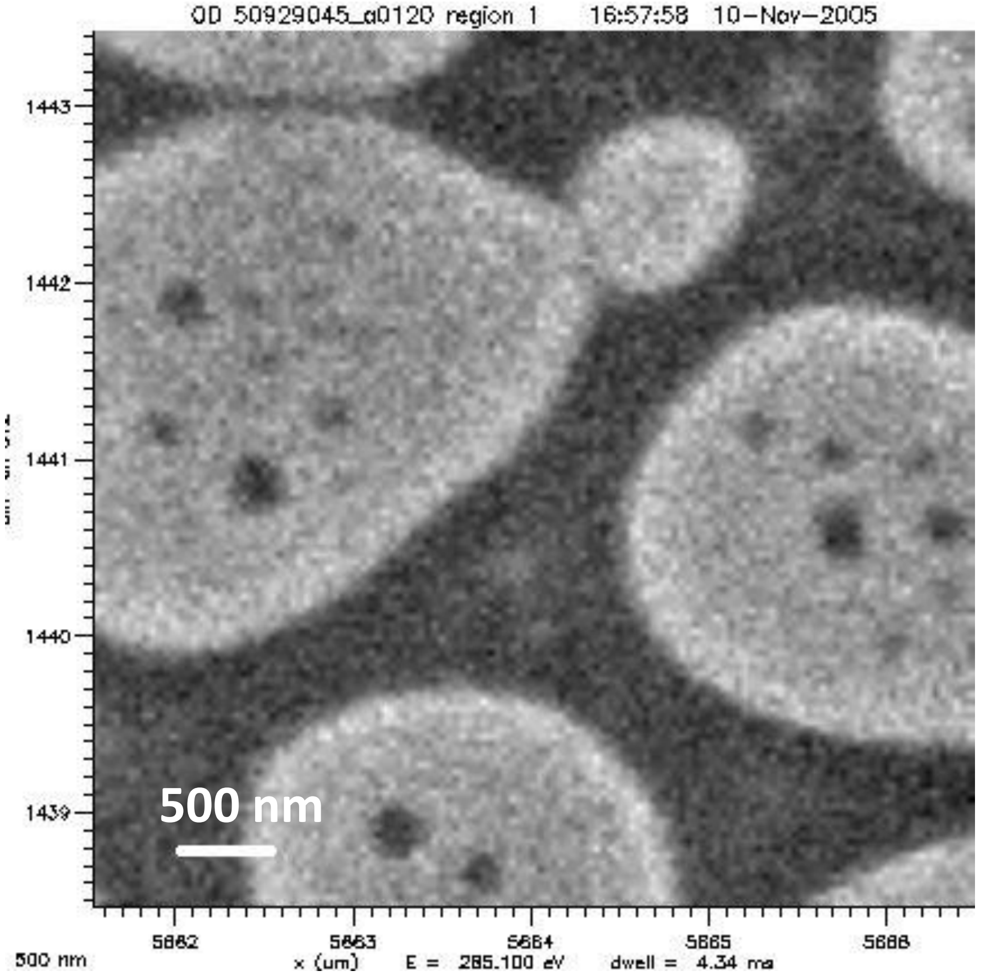
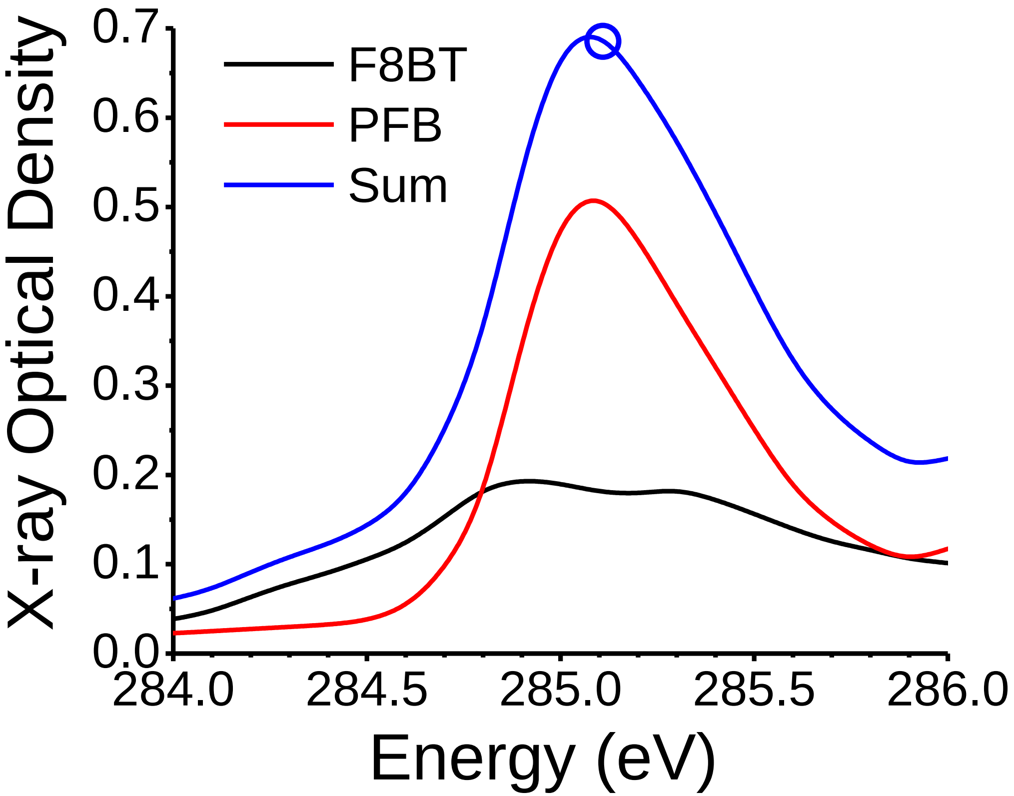
STXM of PFB:F8BT Blends





X-ray Energy (eV): 285.1

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

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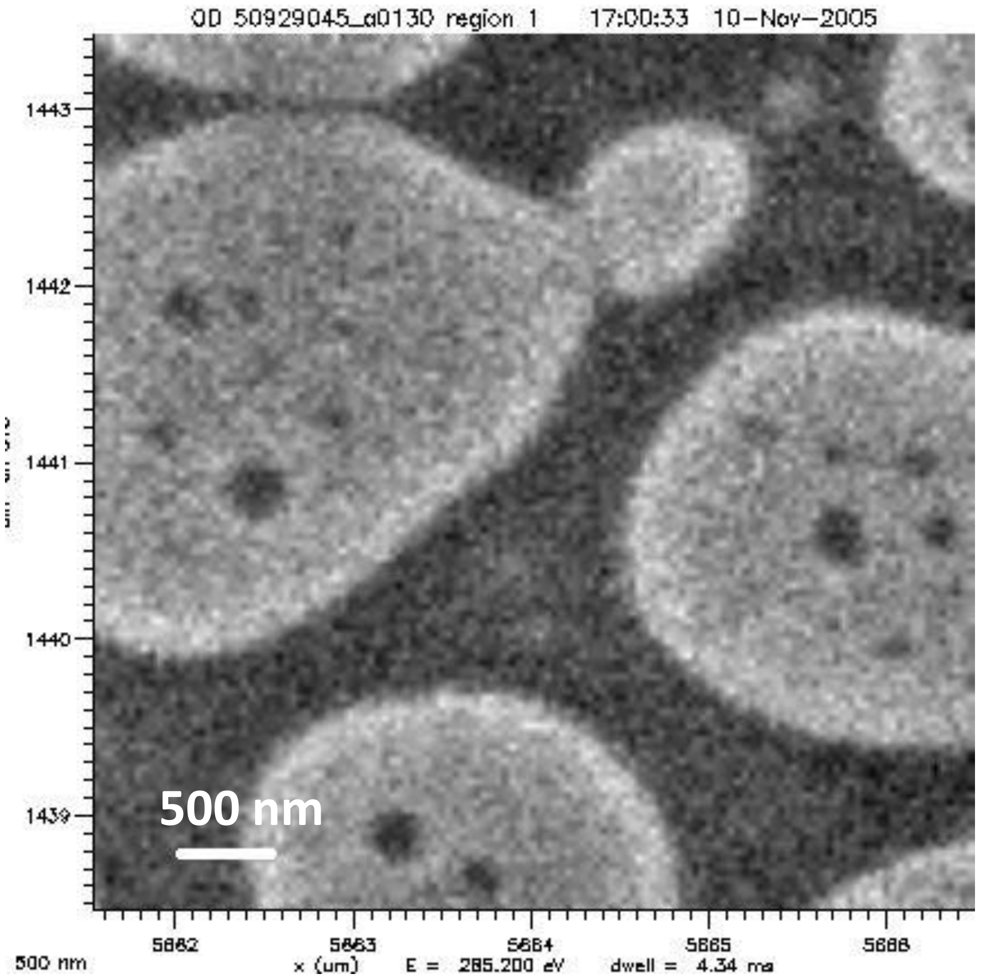
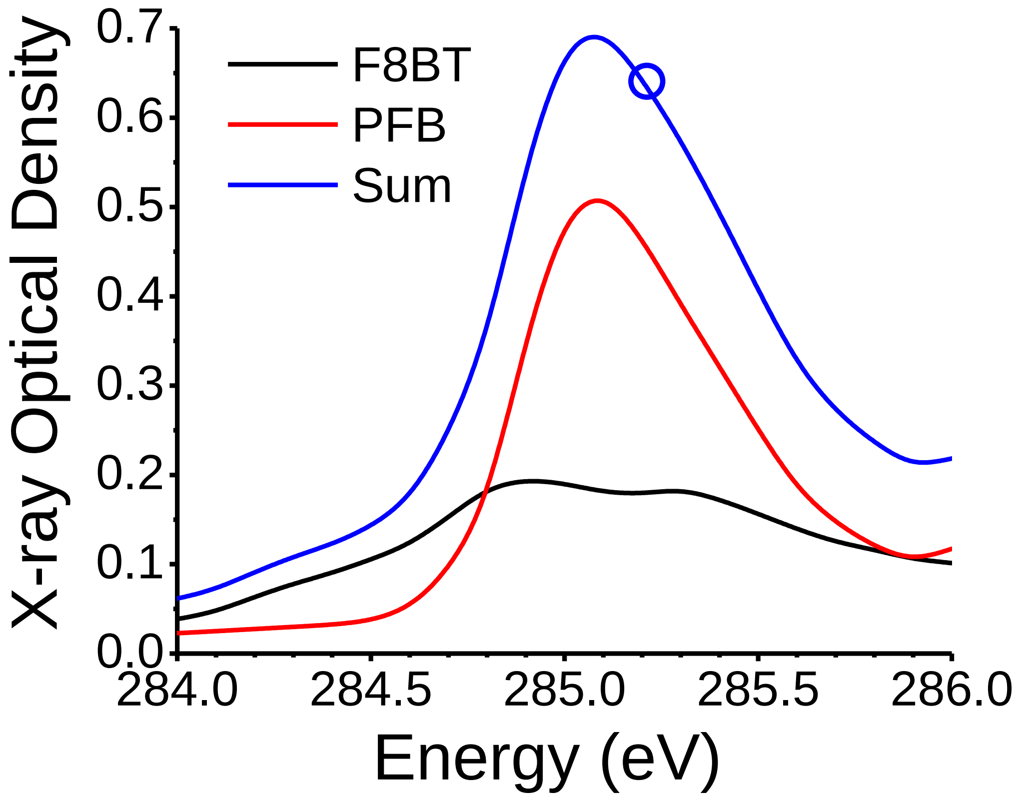
STXM of PFB:F8BT Blends





X-ray Energy (eV): 285.2

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

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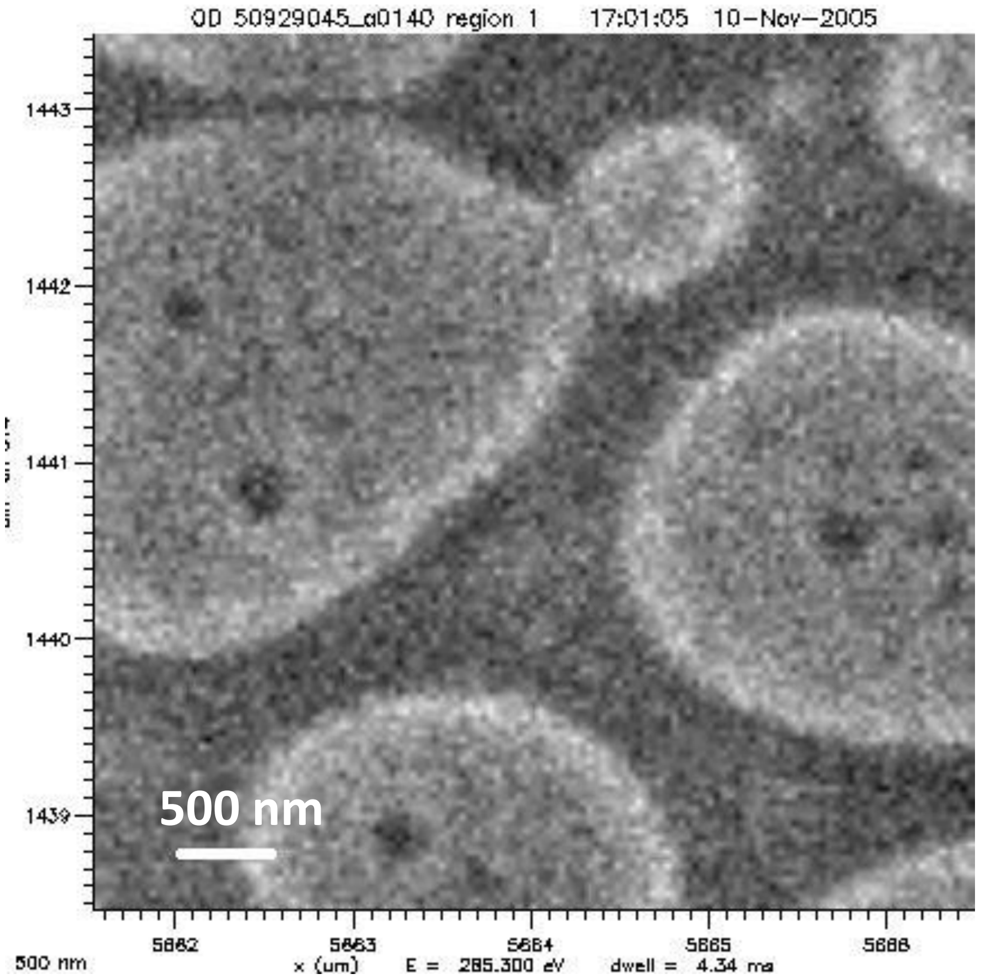
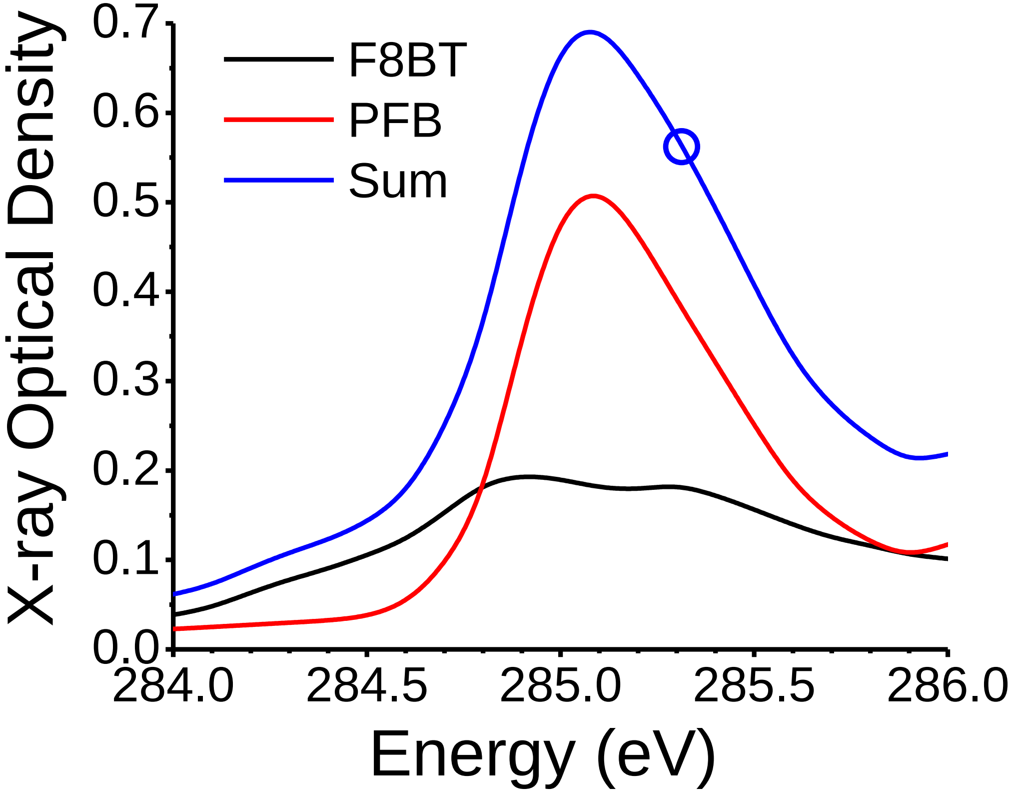
STXM of PFB:F8BT Blends





X-ray Energy (eV): 285.3

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

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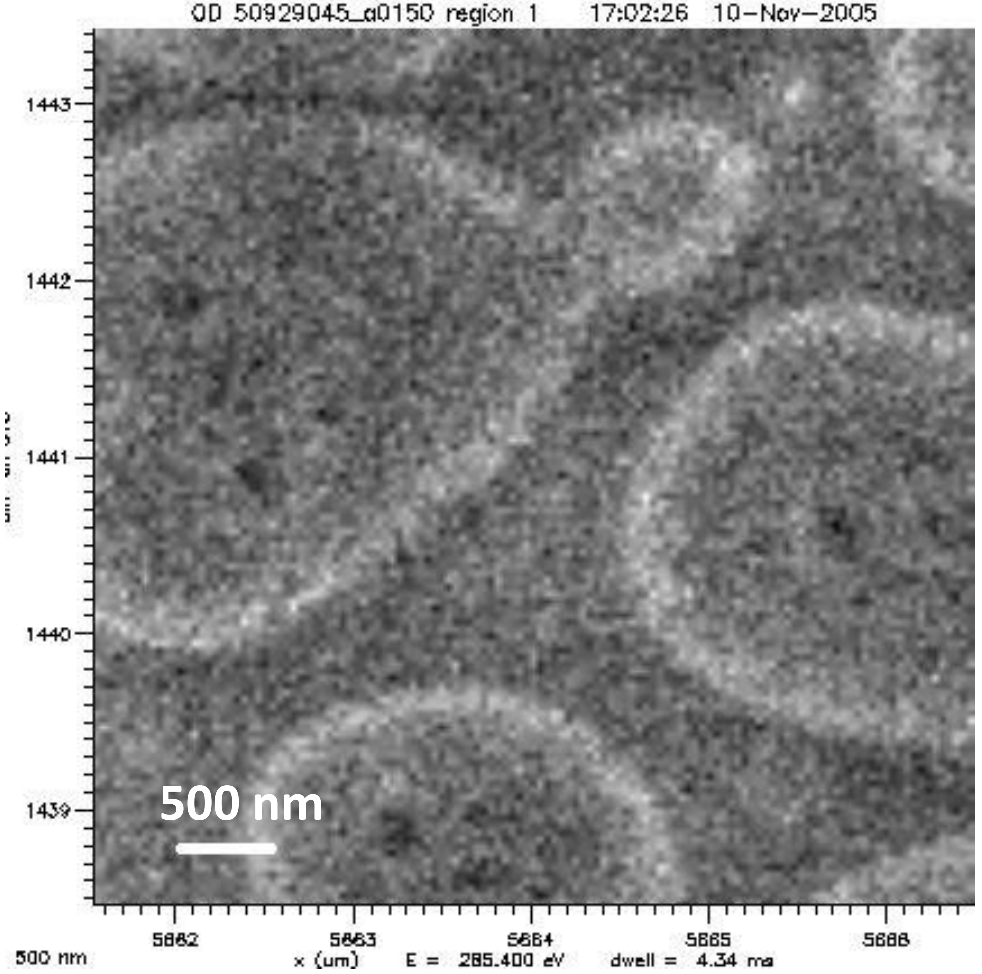
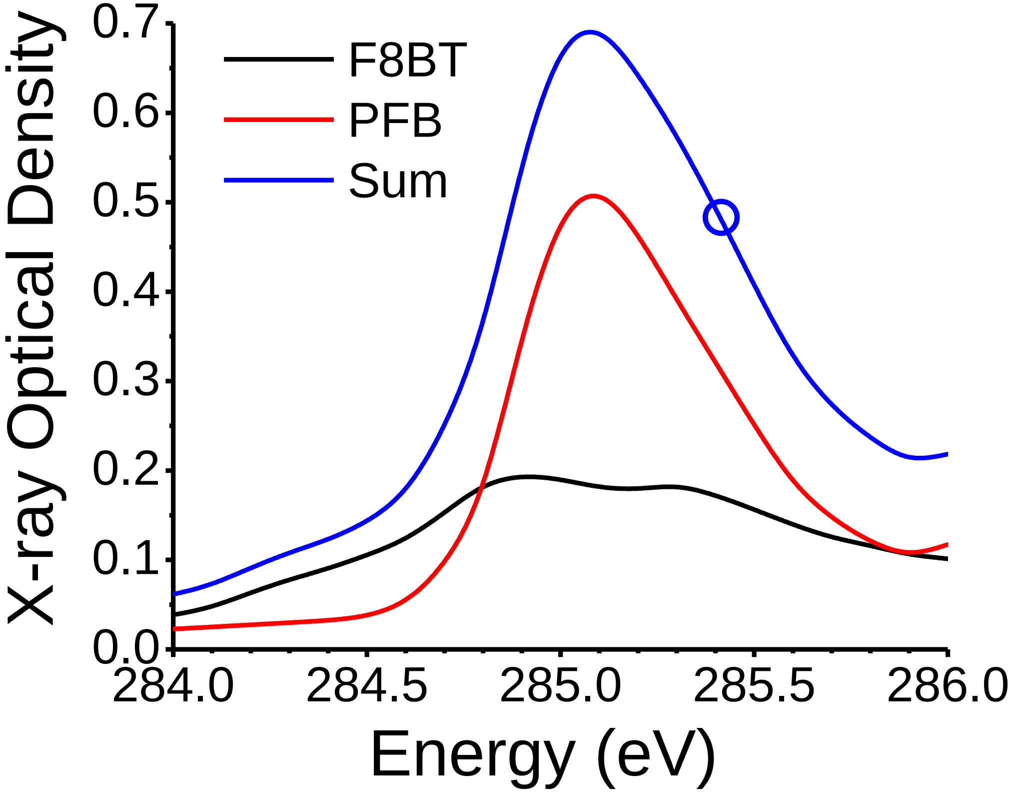
STXM of PFB:F8BT Blends





X-ray Energy (eV): 285.4

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

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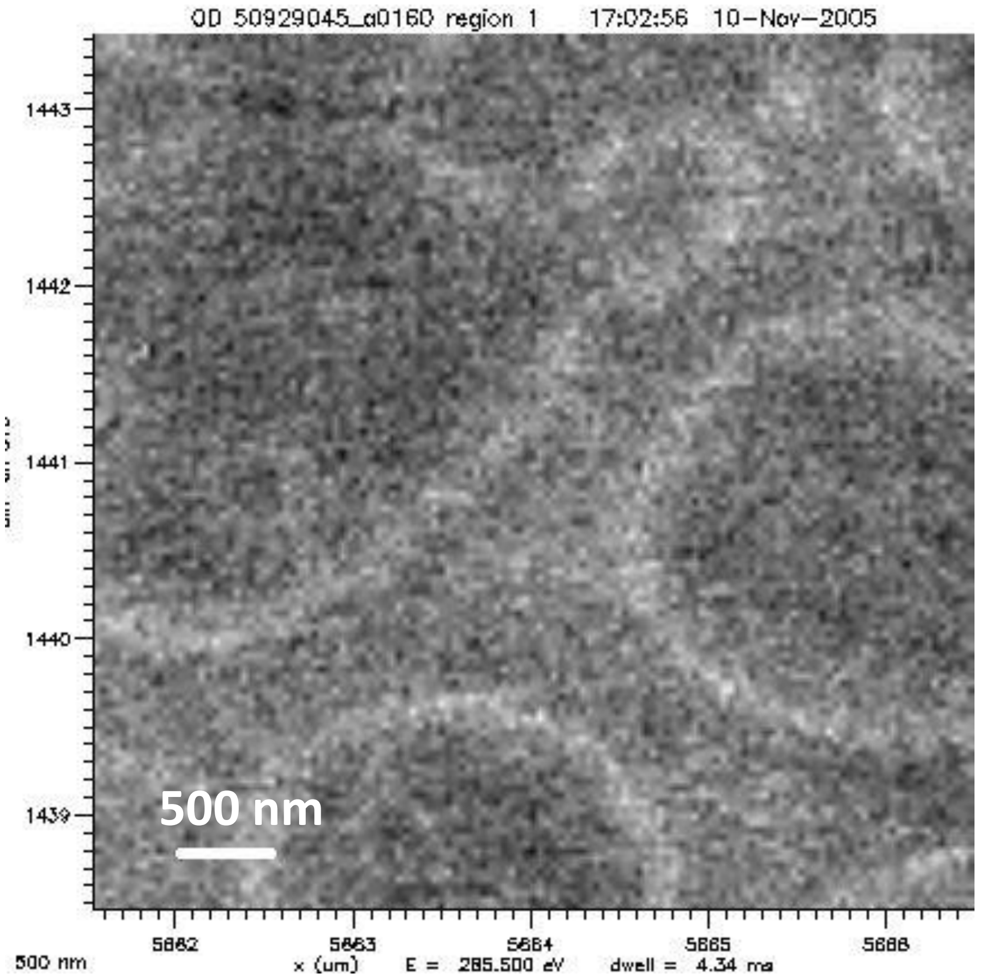
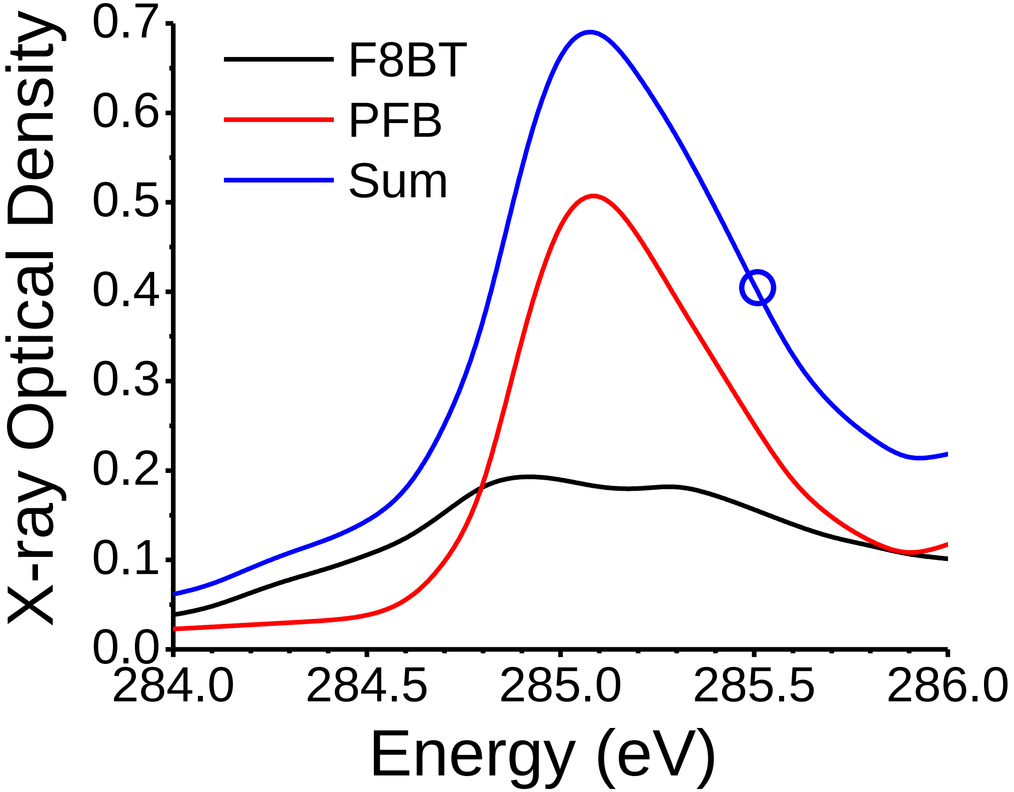
STXM of PFB:F8BT Blends

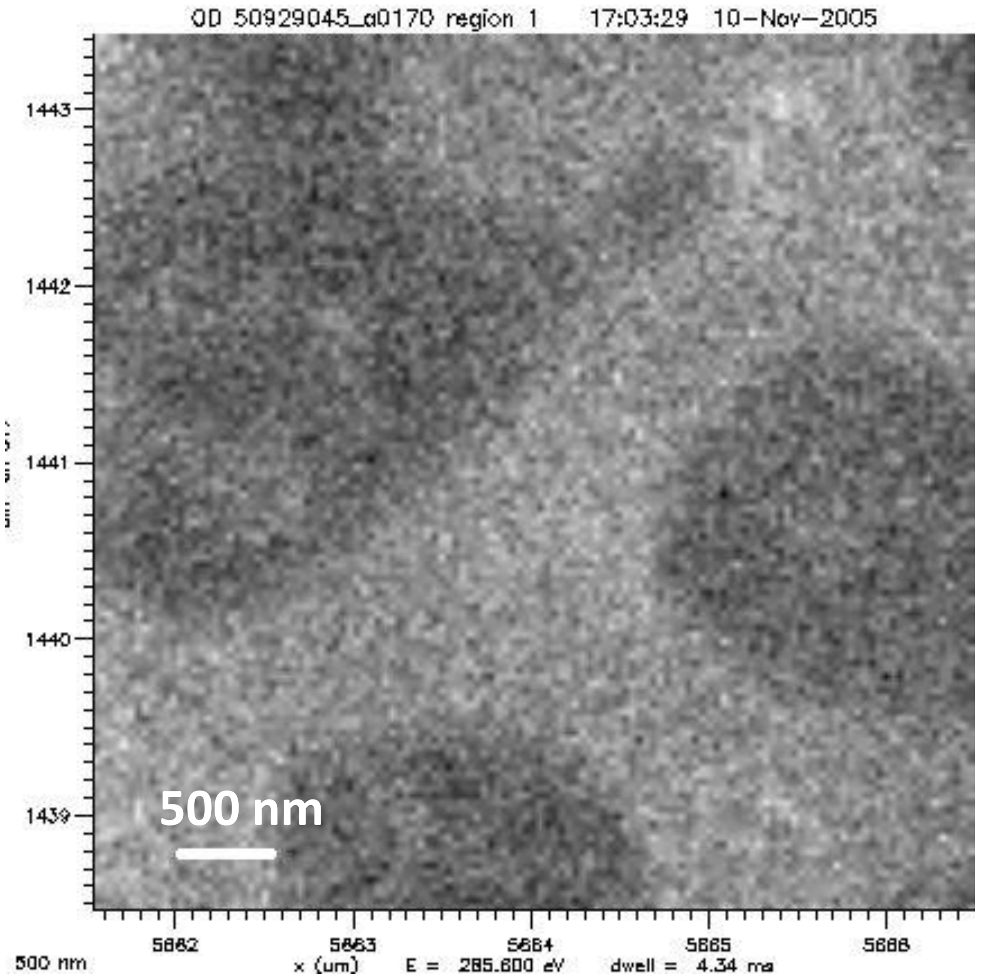


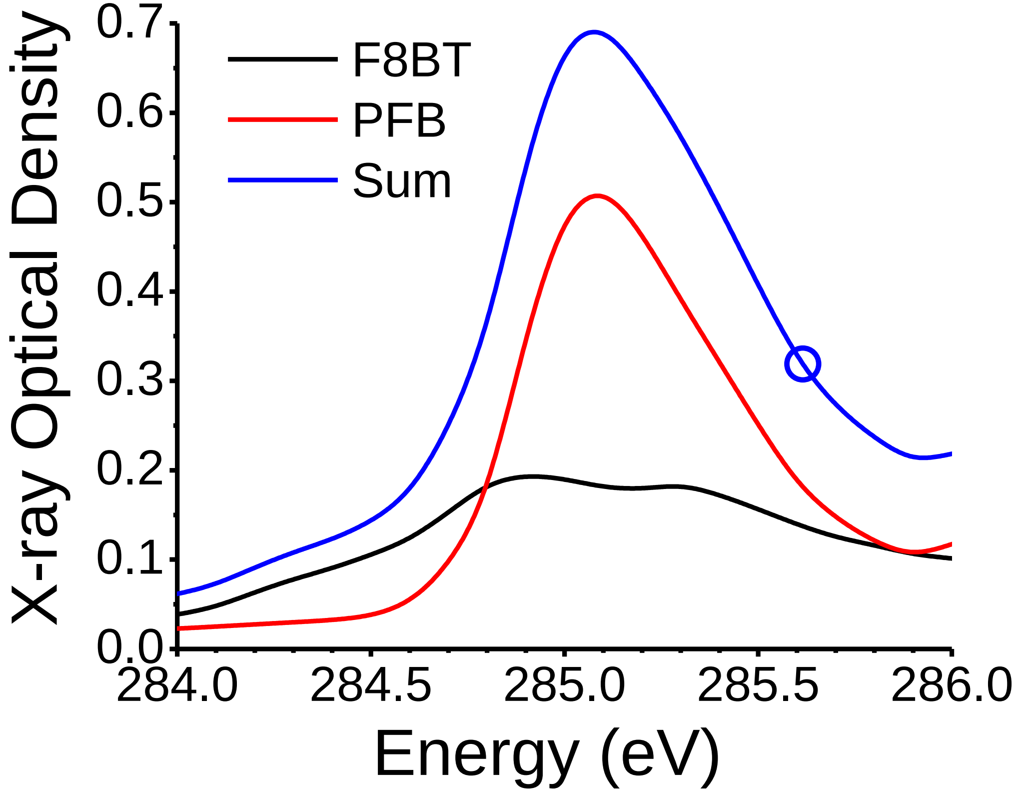


X-ray Energy (eV): 285.5

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

STXM of PFB:F8BT Blends





X-ray Energy (eV): 285.6

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

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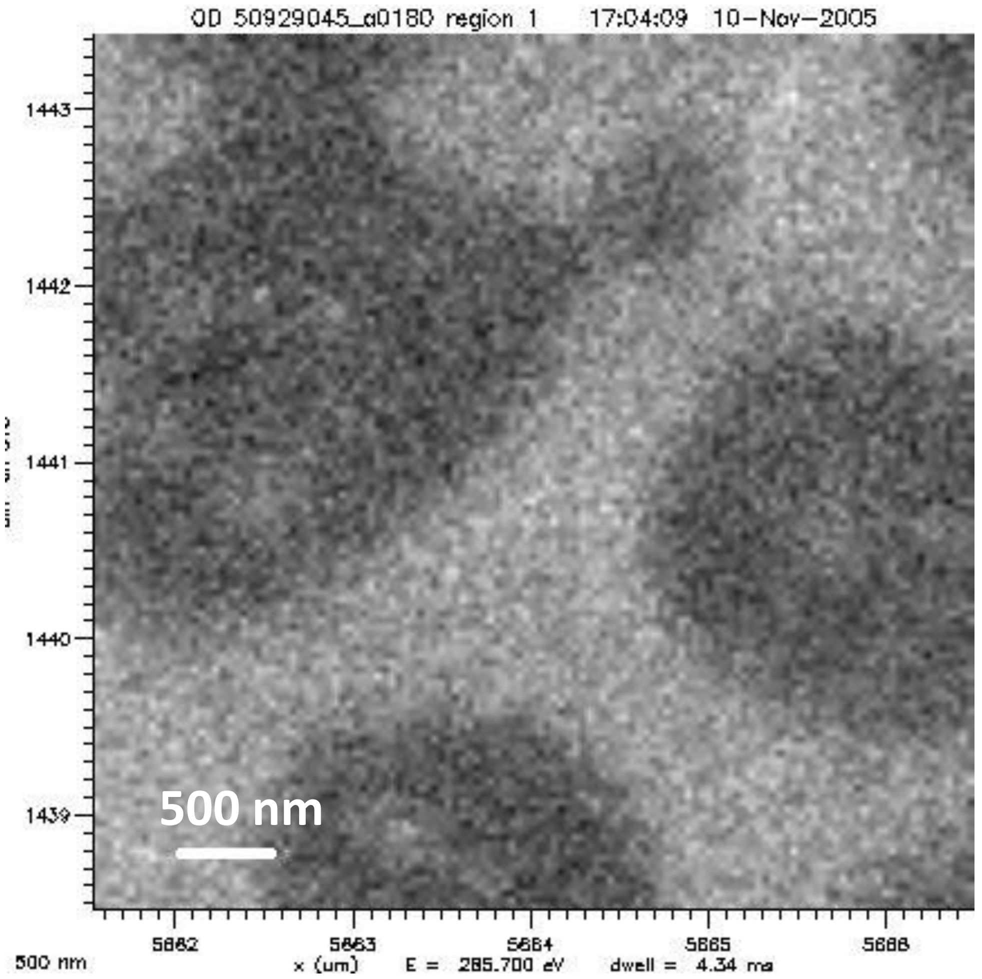
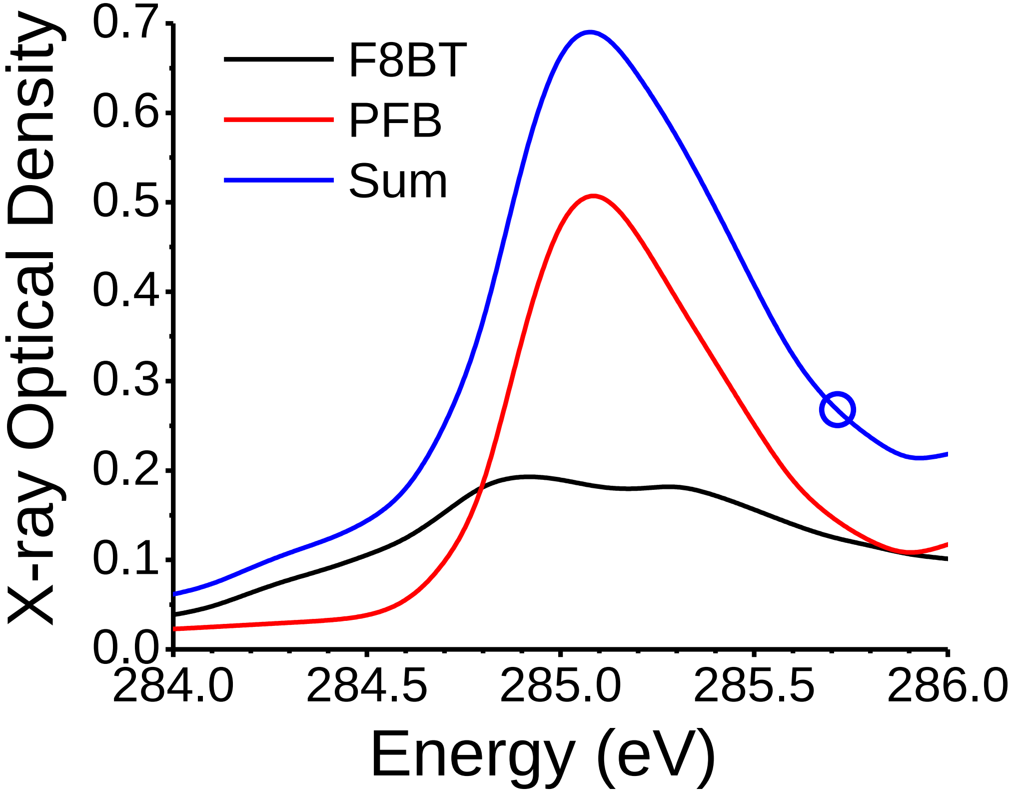
STXM of PFB:F8BT Blends





X-ray Energy (eV): 285.7

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

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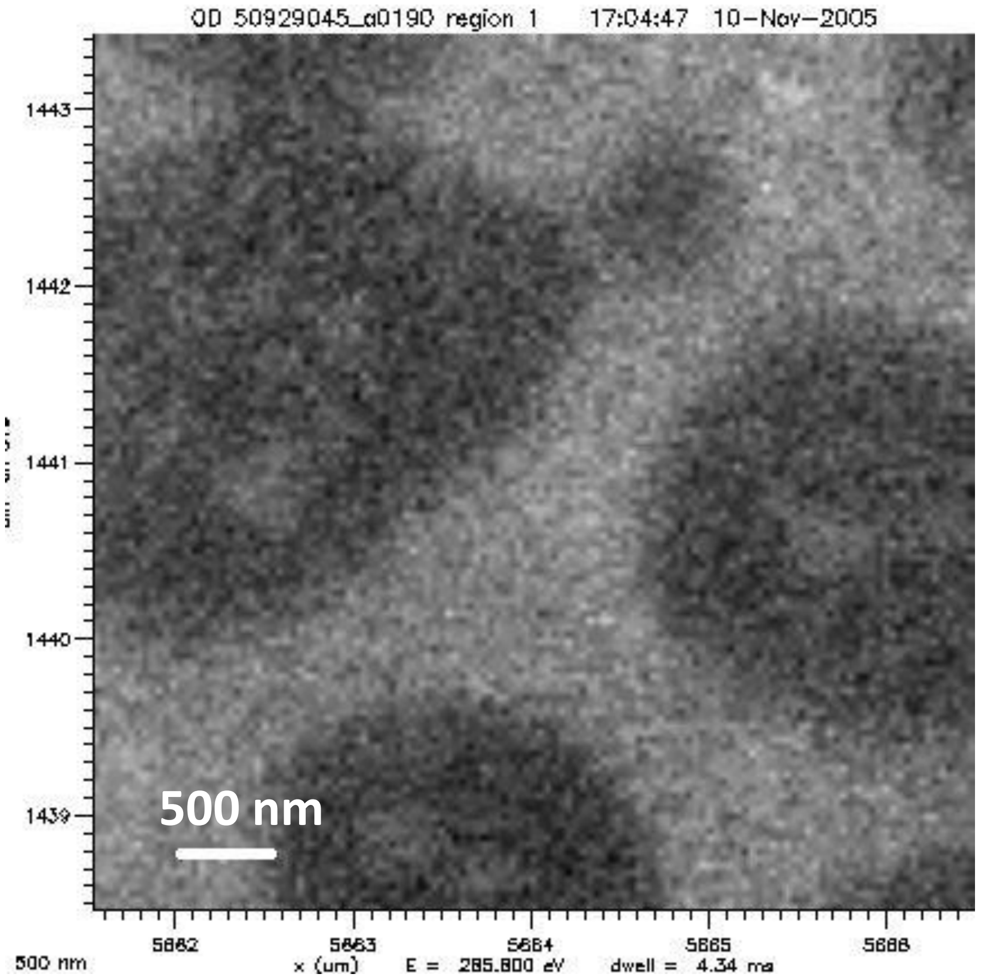
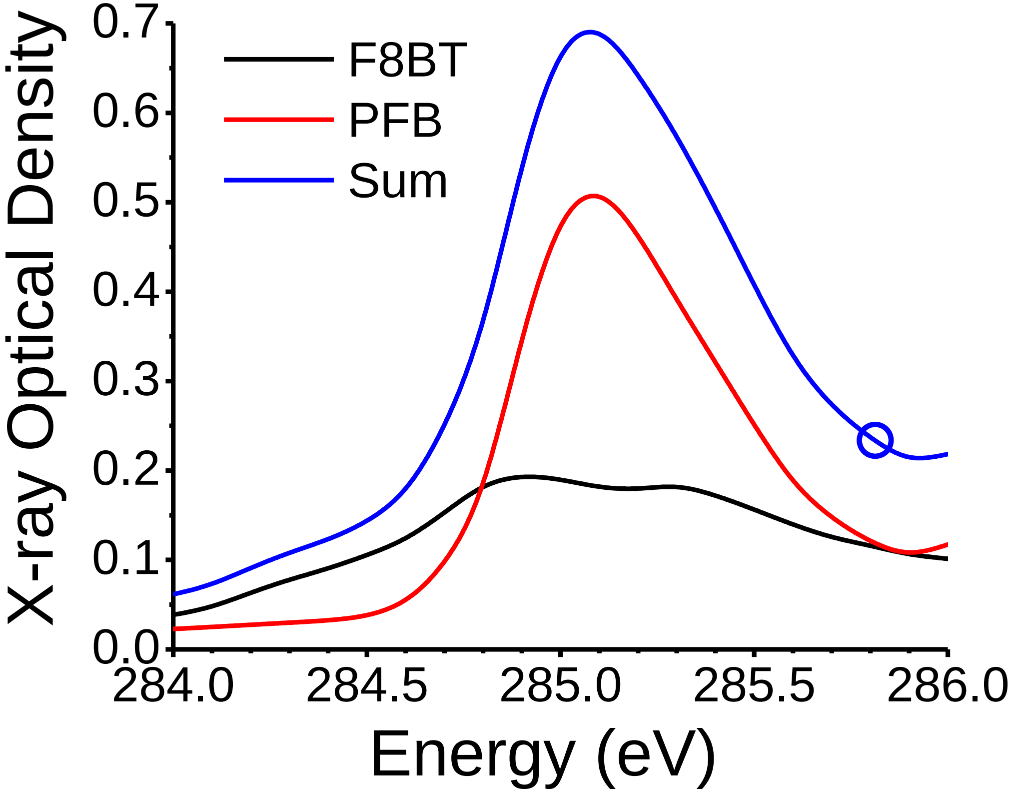
STXM of PFB:F8BT Blends

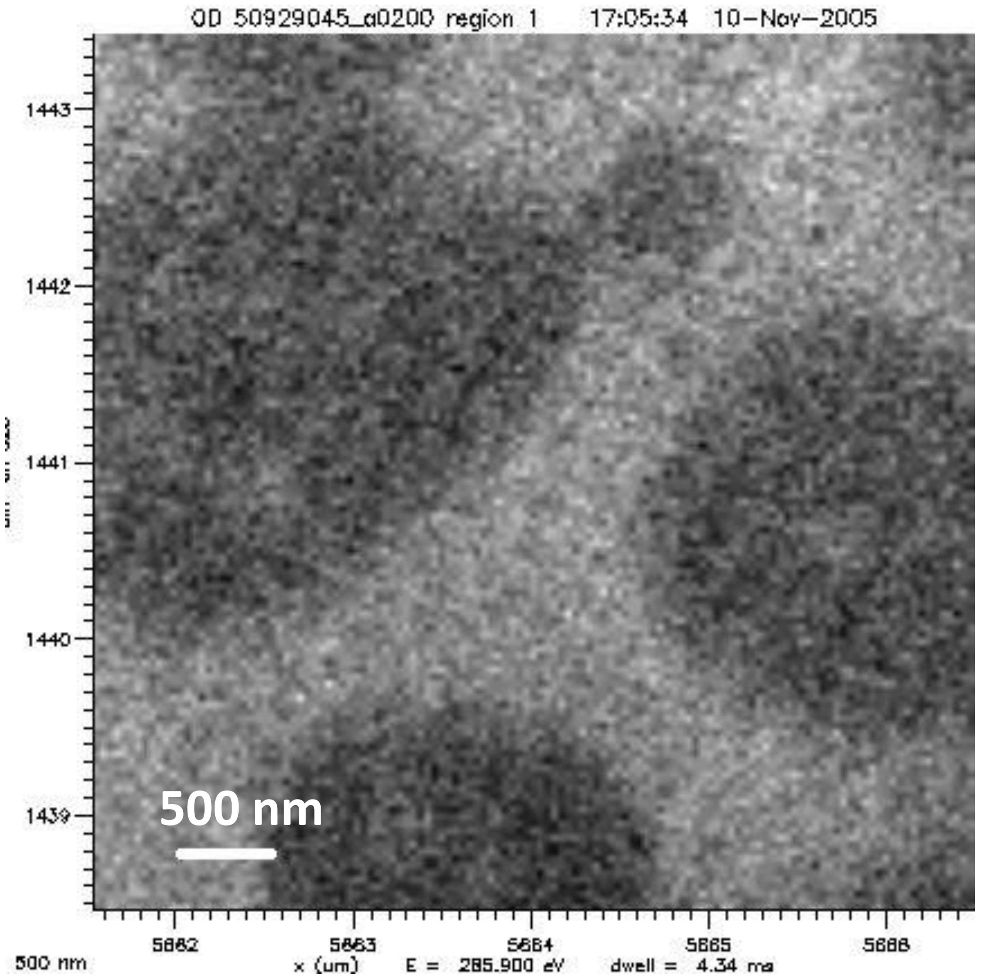


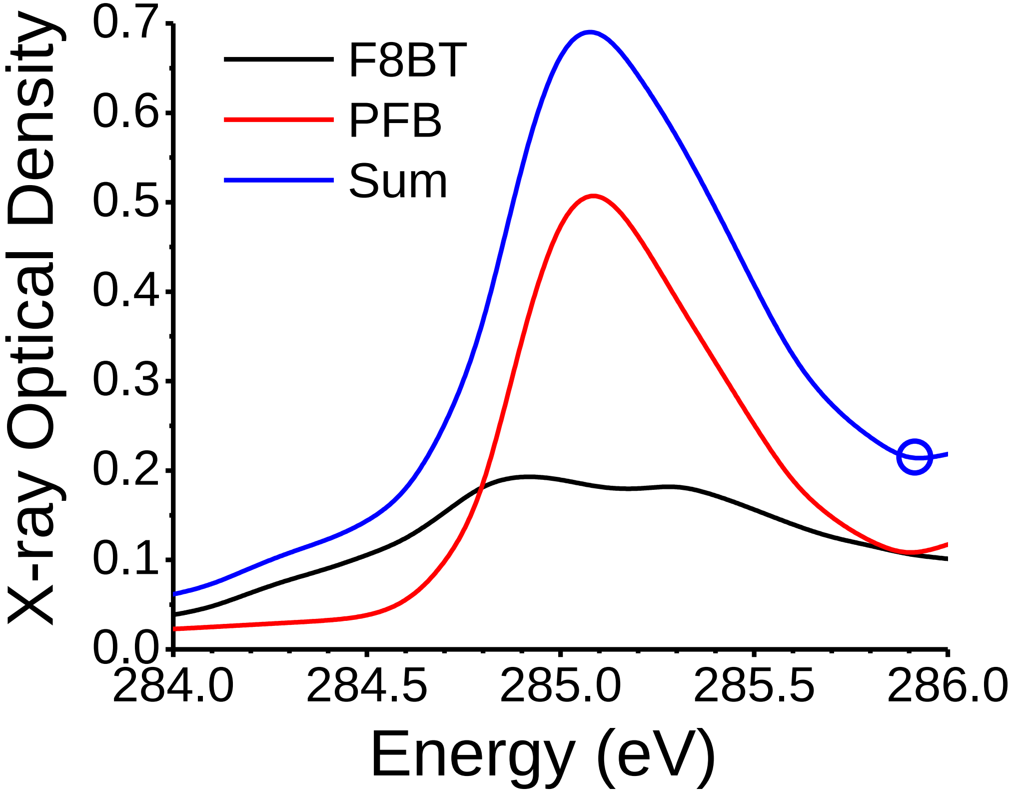


X-ray Energy (eV): 285.8

C. R. McNeill *et al.*, *Nano Lett.* **6**, 1202 (2006).

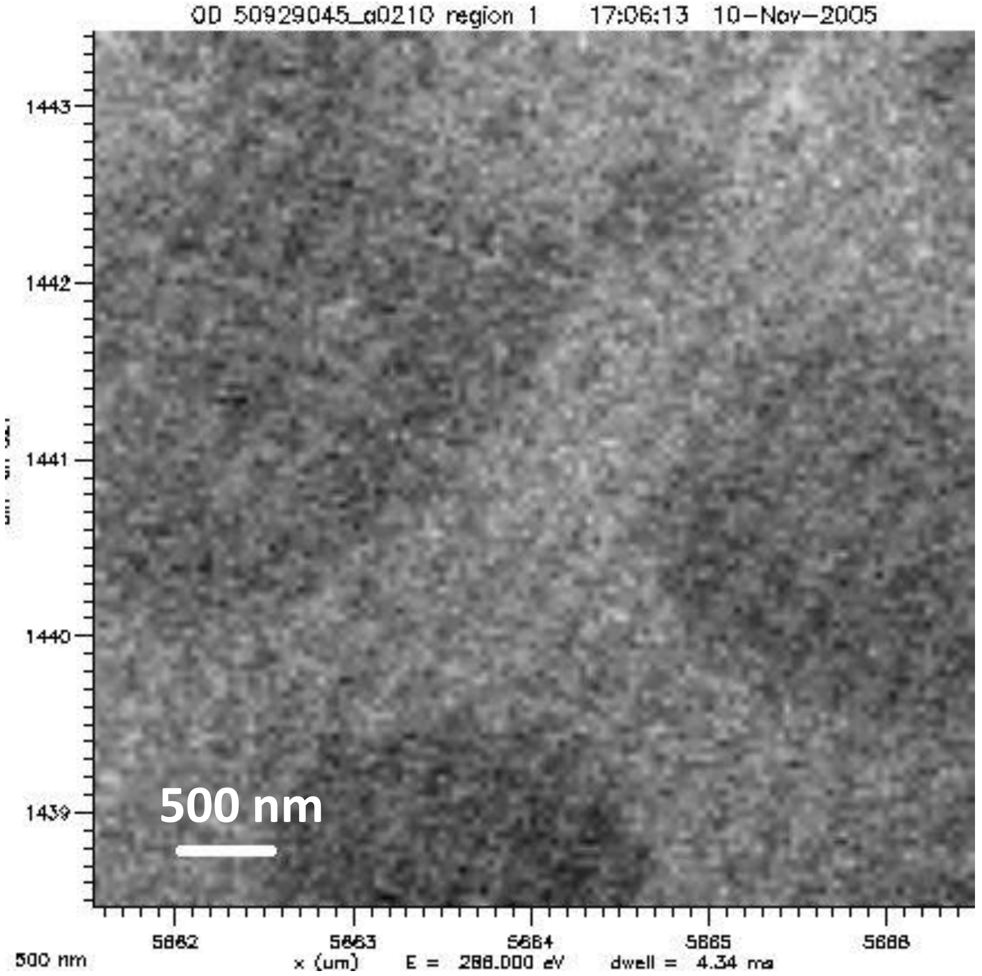
STXM of PFB:F8BT Blends

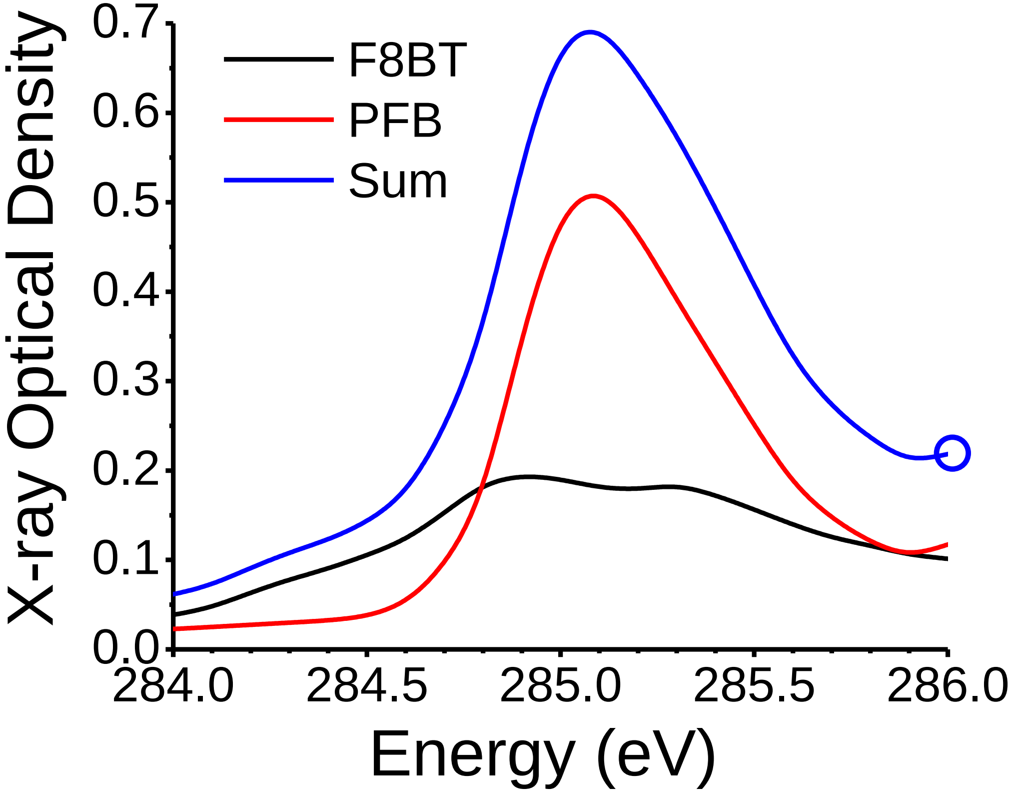




X-ray Energy (eV): 285.9

STXM of PFB:F8BT Blends

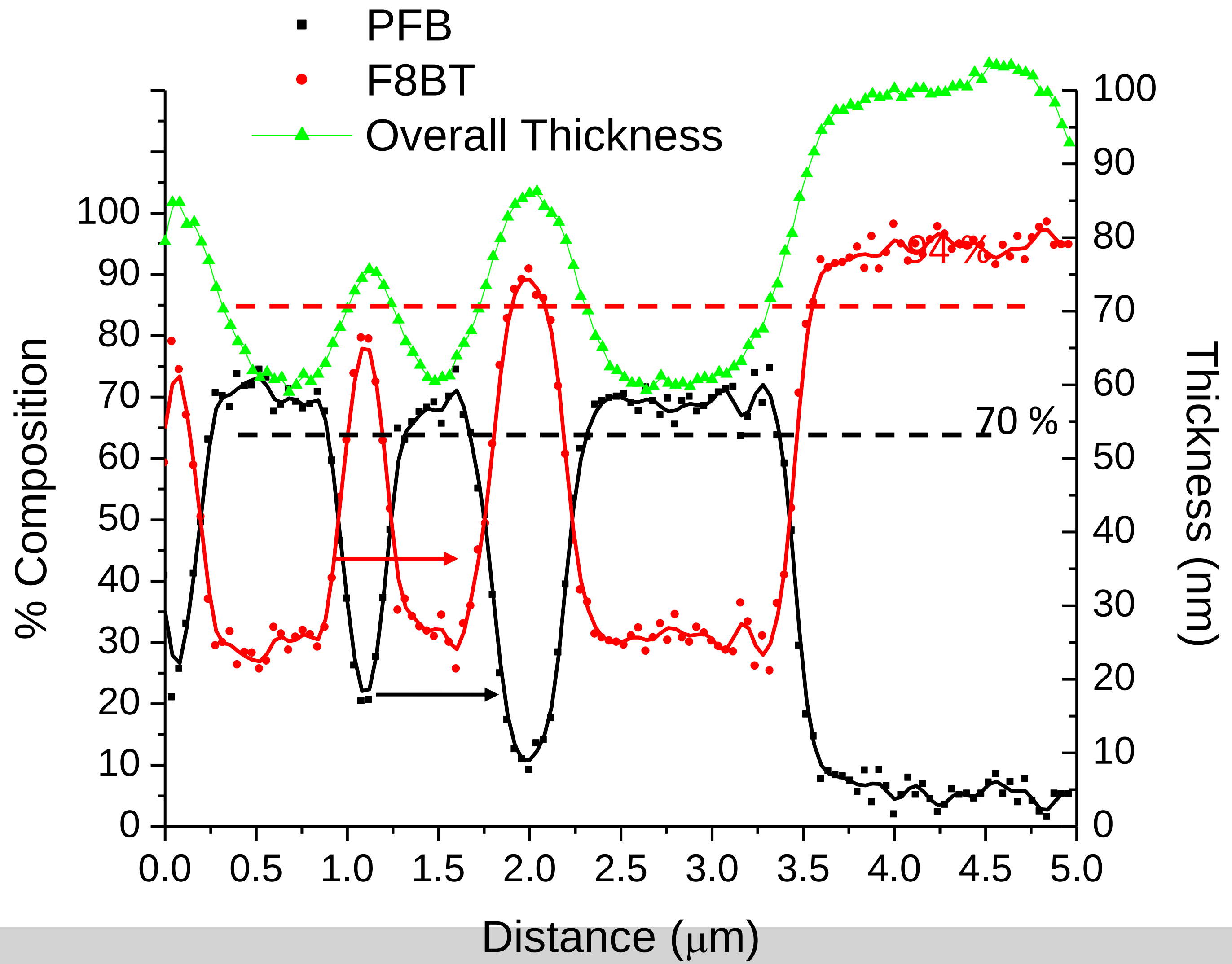


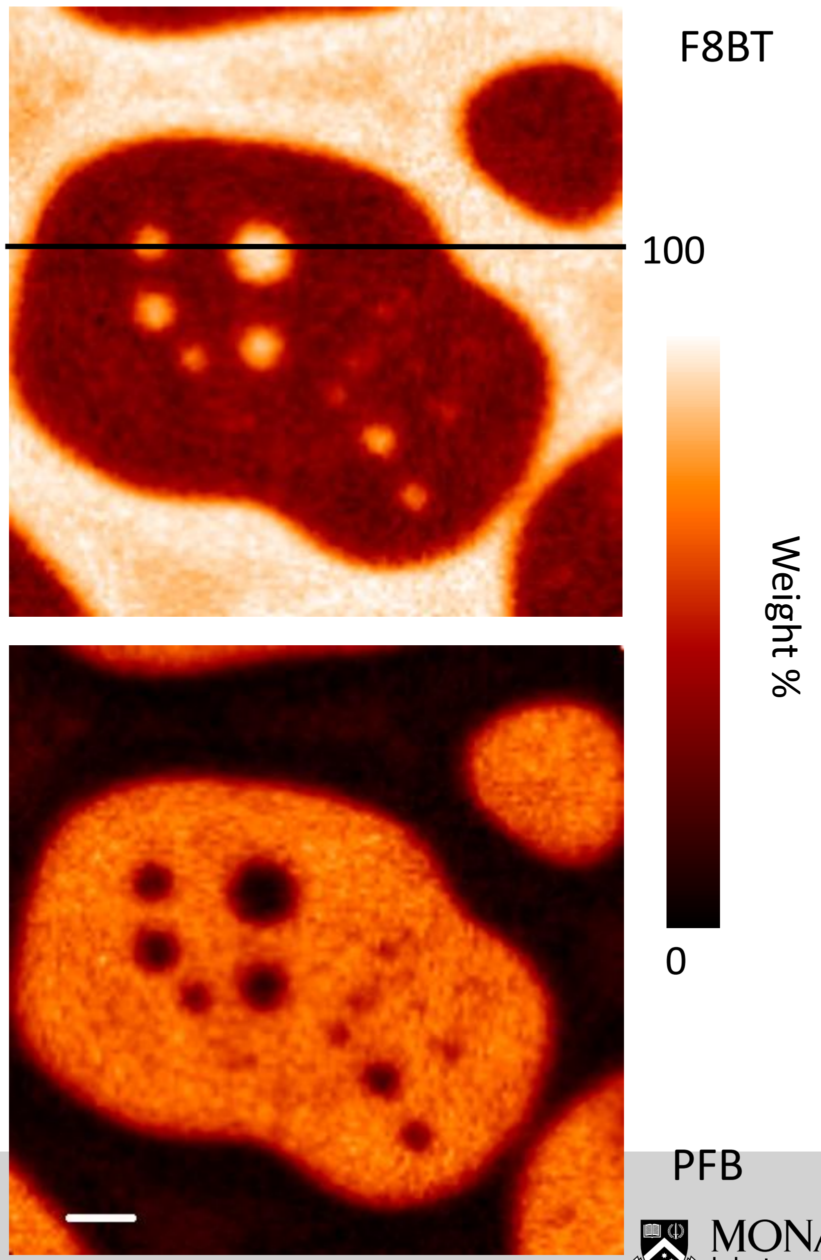


X-ray Energy (eV): 286.0

C. R. McNeill *et al., Nano Lett.* **6**, 1202 (2006).

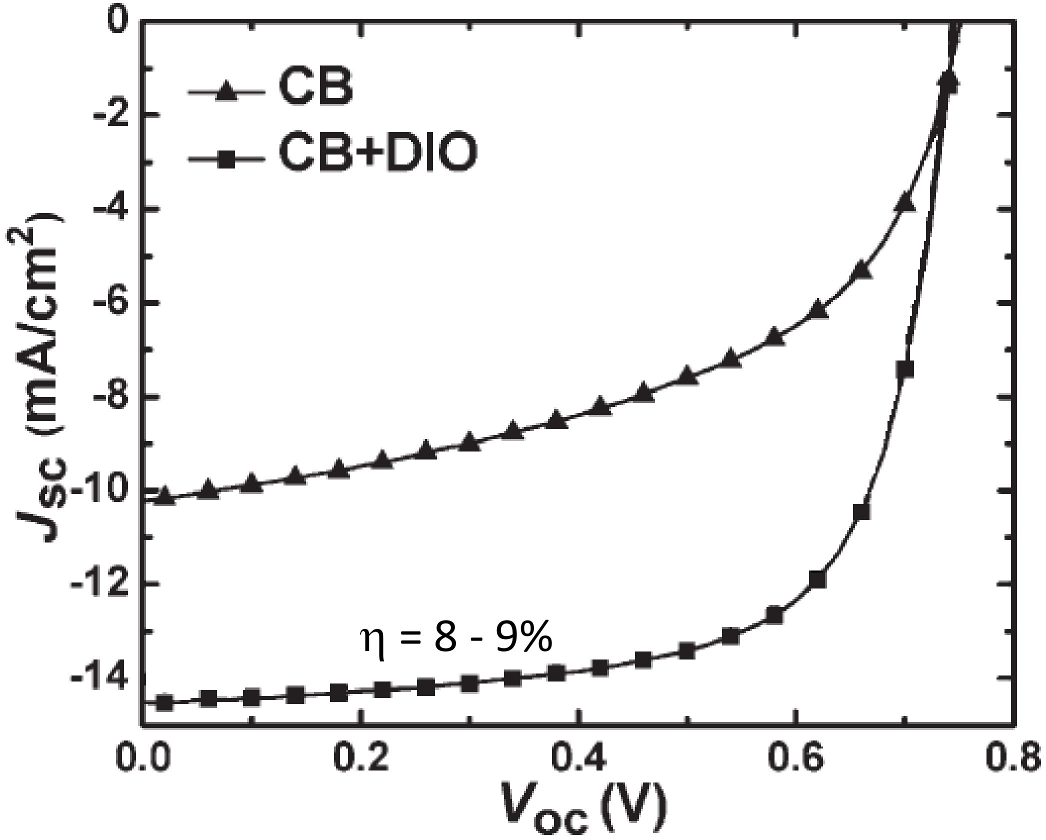
STXM of PFB:F8BT Blends

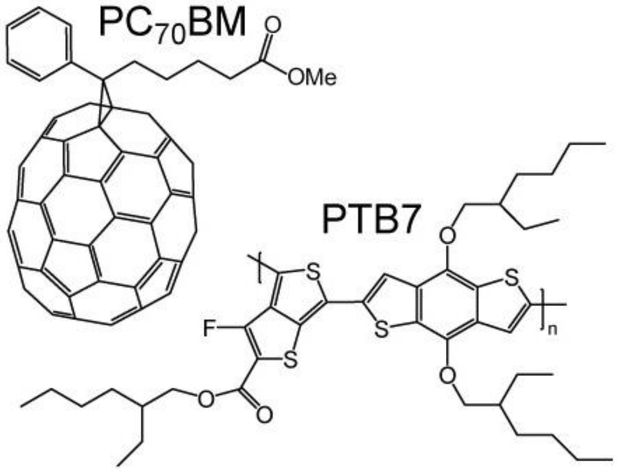


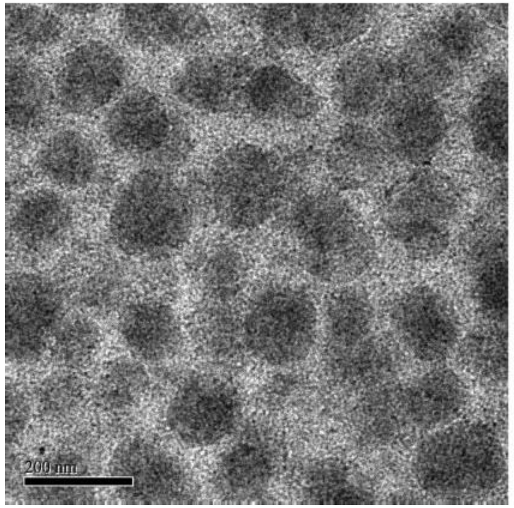


McNeill et al., *Macromolecules* **40**, 3263 (2007).

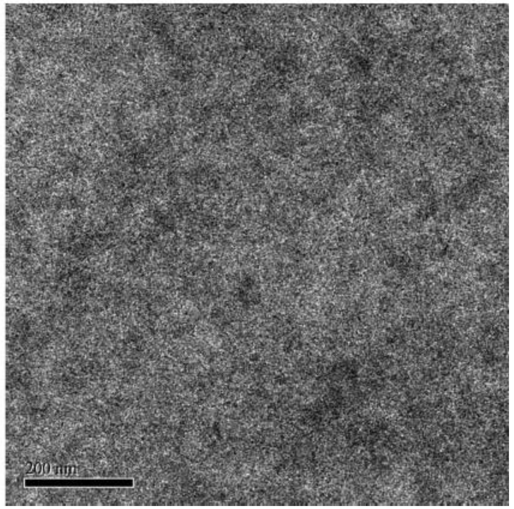
PTB7:$PC_{70}BM$







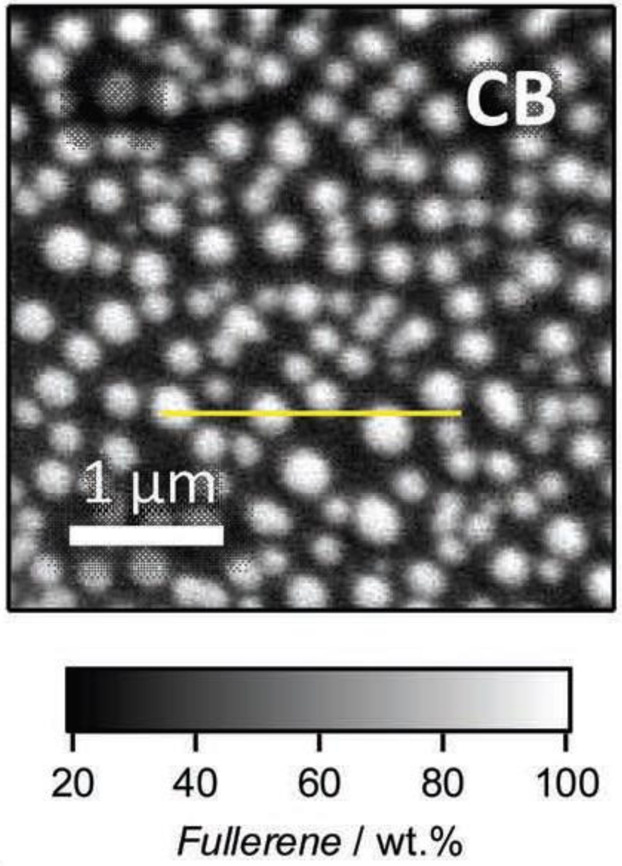
Without DIO

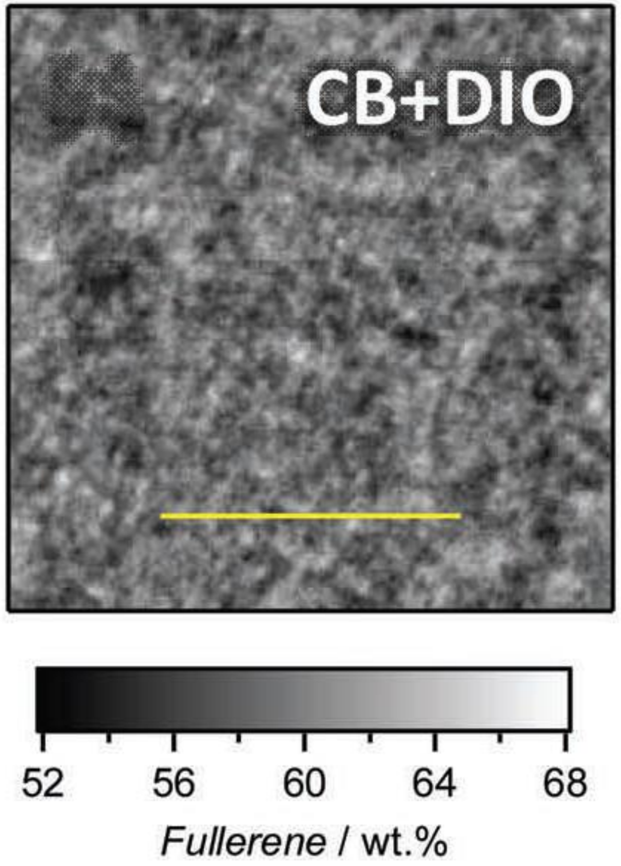


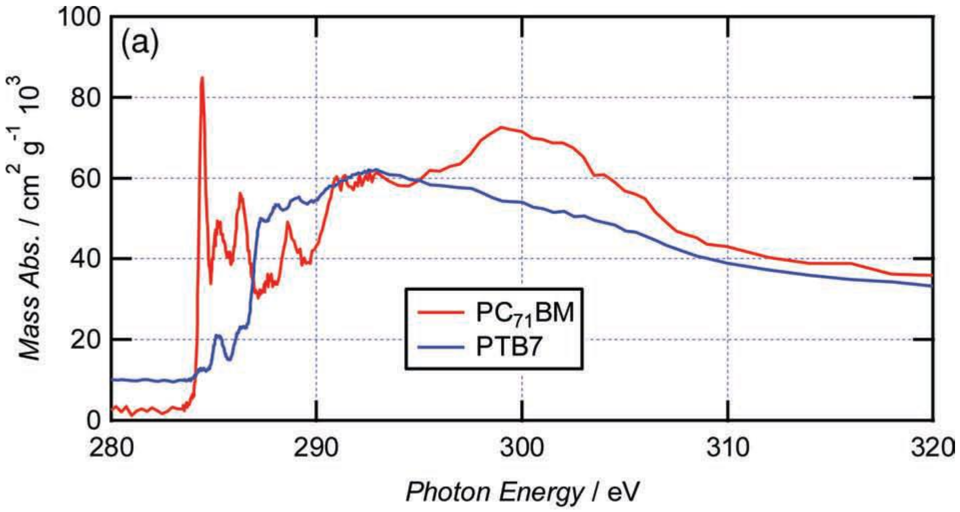
With DIO

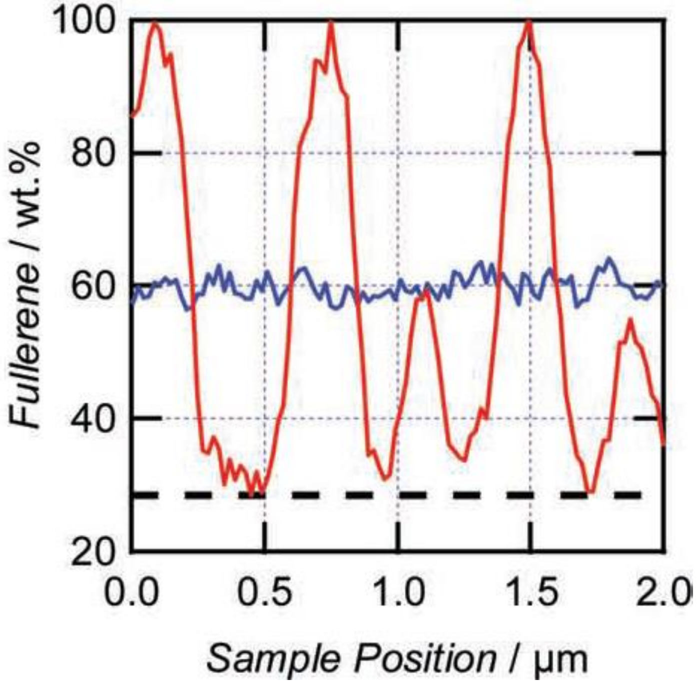
Liang et al. *Adv. Mater.* **22,** E135 - E138 (2010).

PTB7:PC_{70}BM









Collins et al. *Adv. Energy Mater.* **3** 65 - 74**,** (2013)

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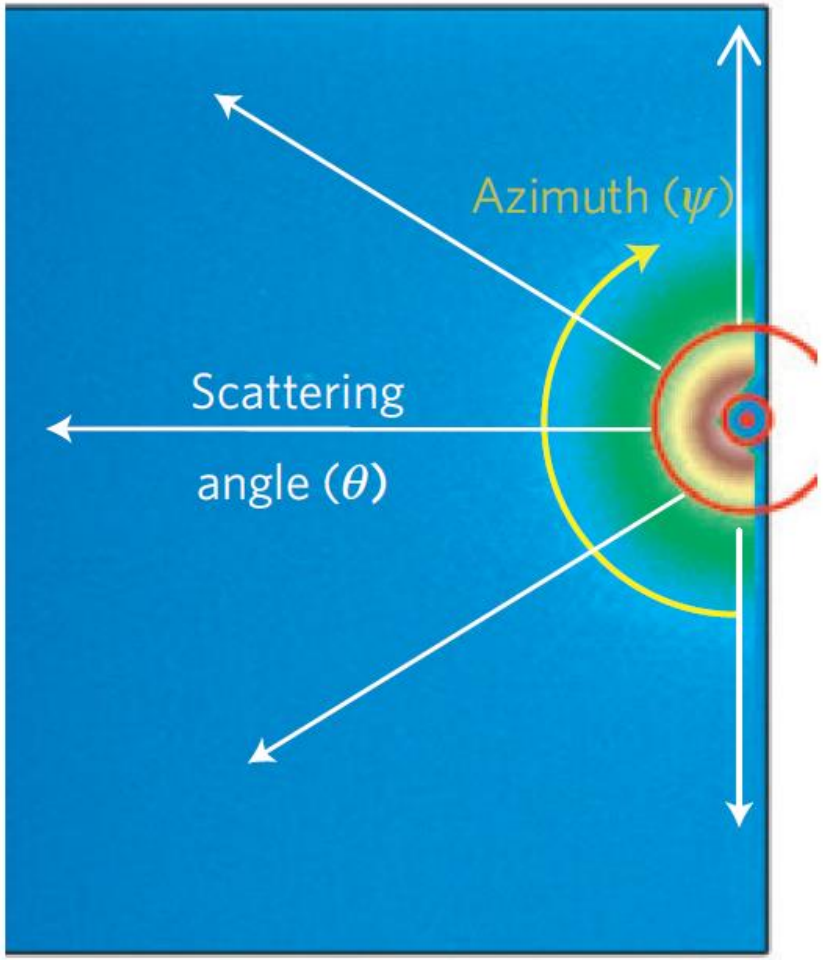
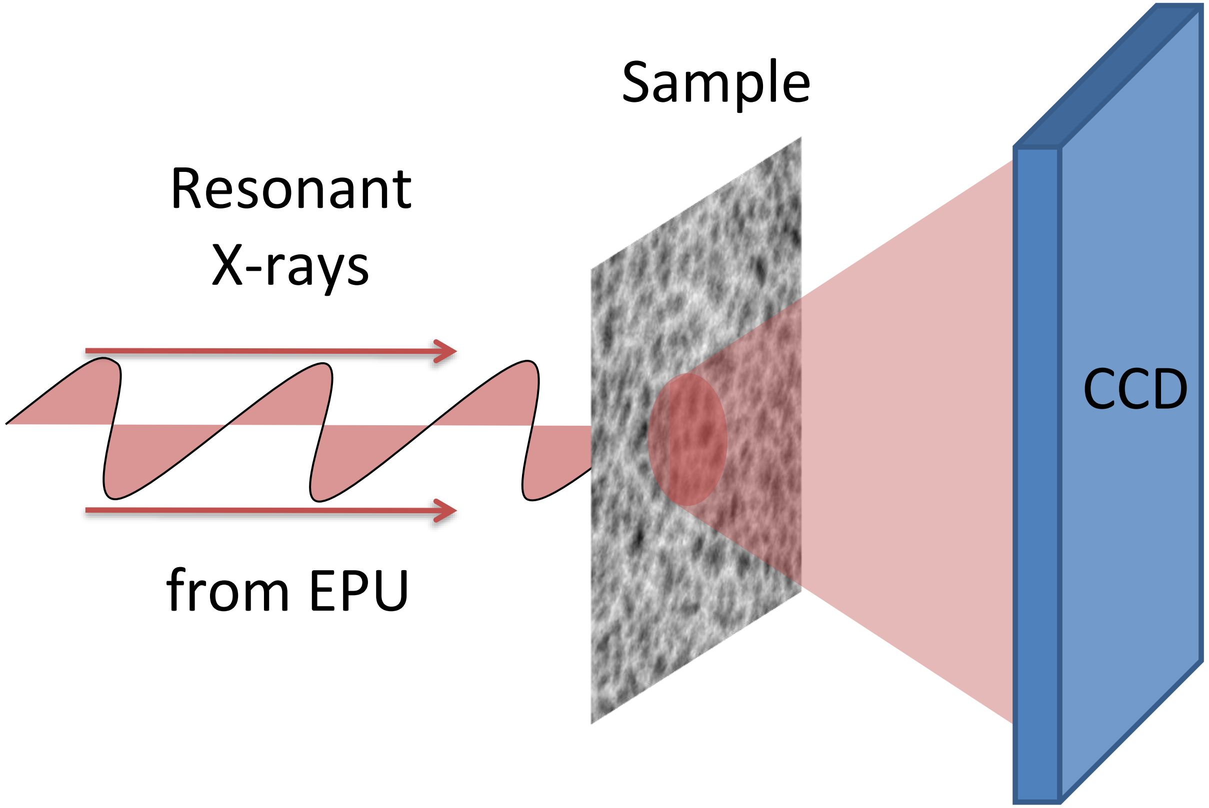
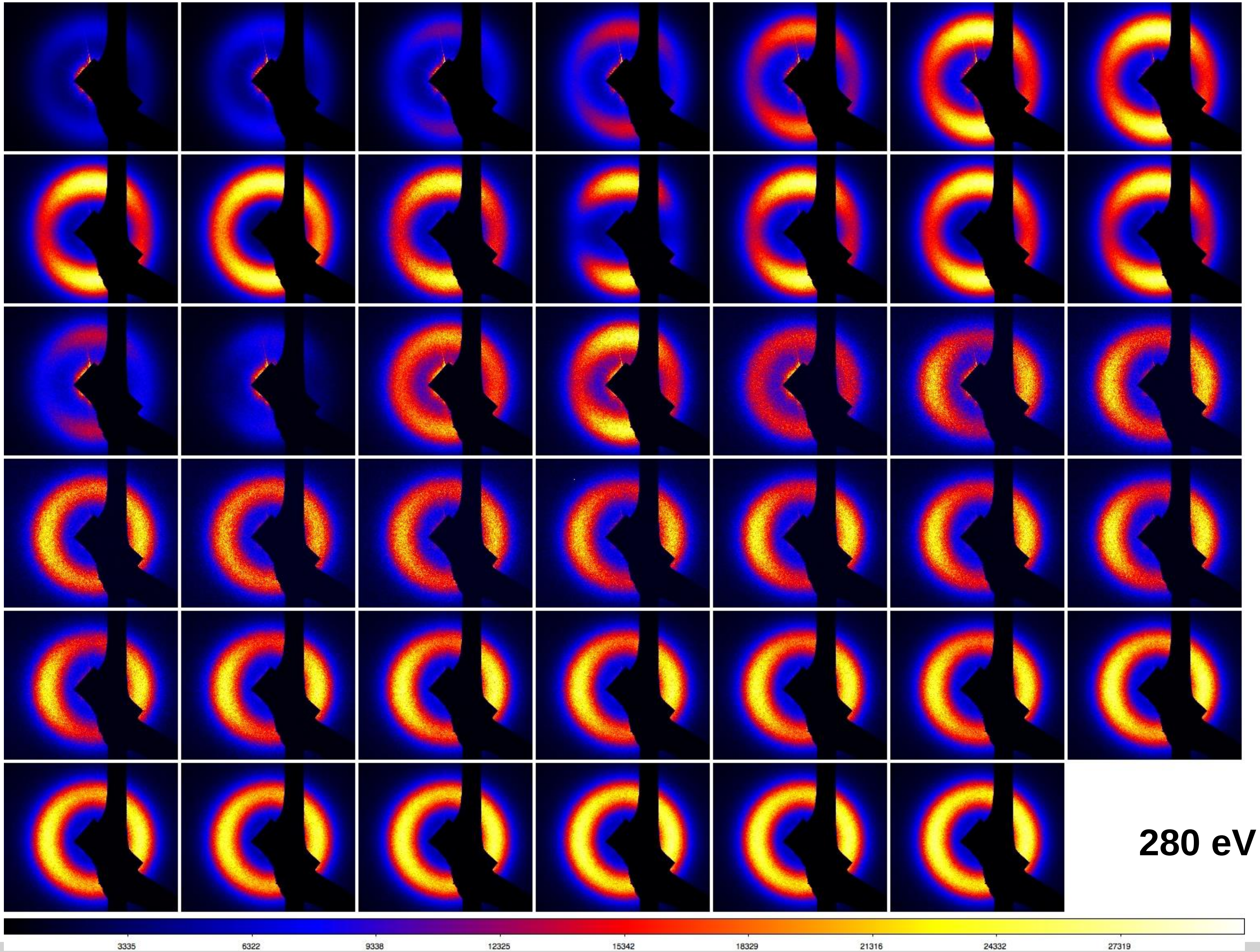
STXM → R-SoXS



Azimuth (ψ)
Scattering
angle (θ)



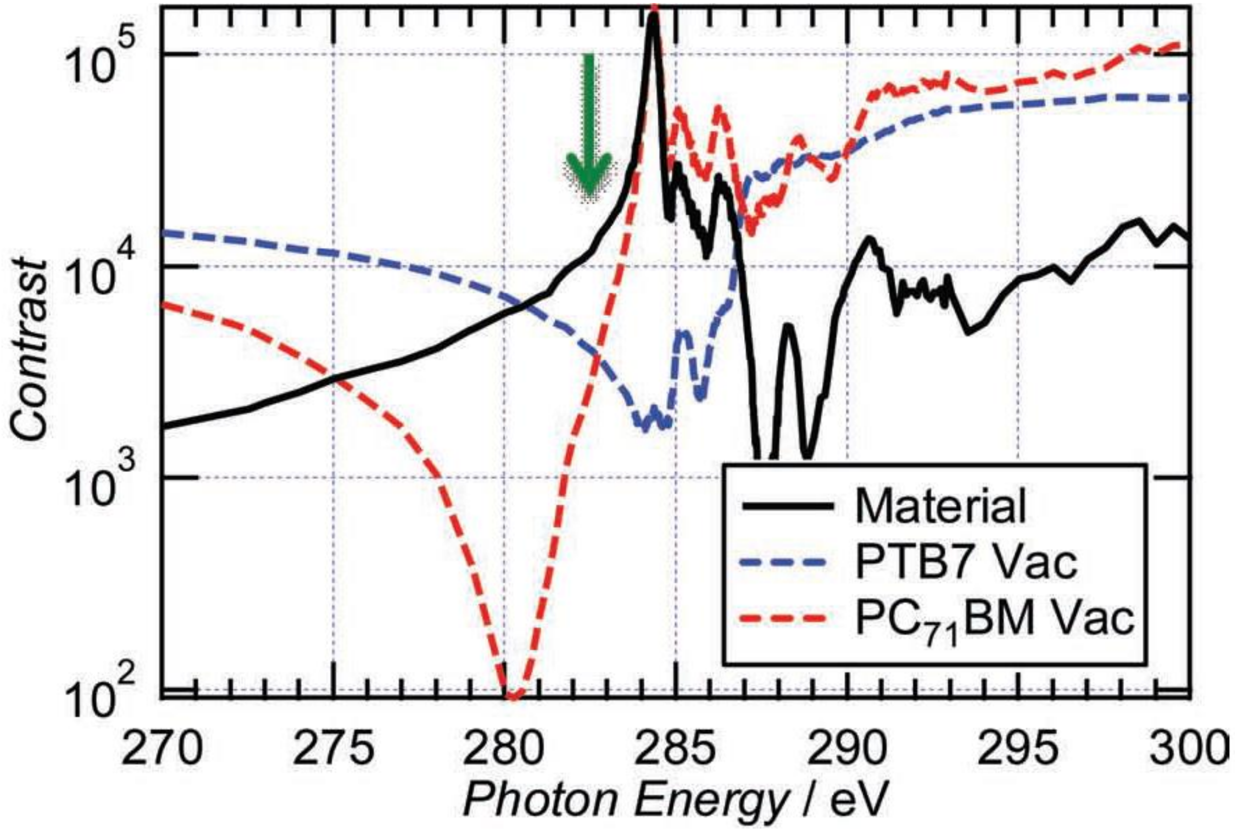
Sample
Resonant
X-rays
from EPU
CCD



280 eV – 300 eV

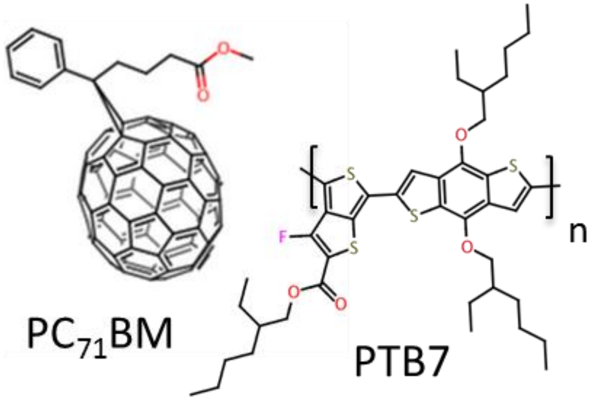
R-SoXS Contrast

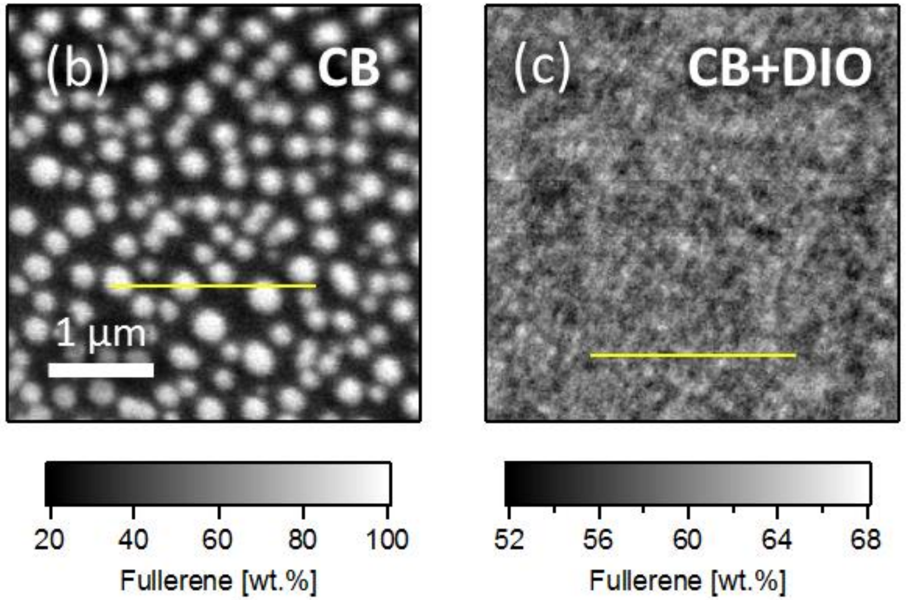
$$I(E) \propto F^2(E) \propto E^4 \,|\, \delta(E) + i\beta(E) \,|^2$$

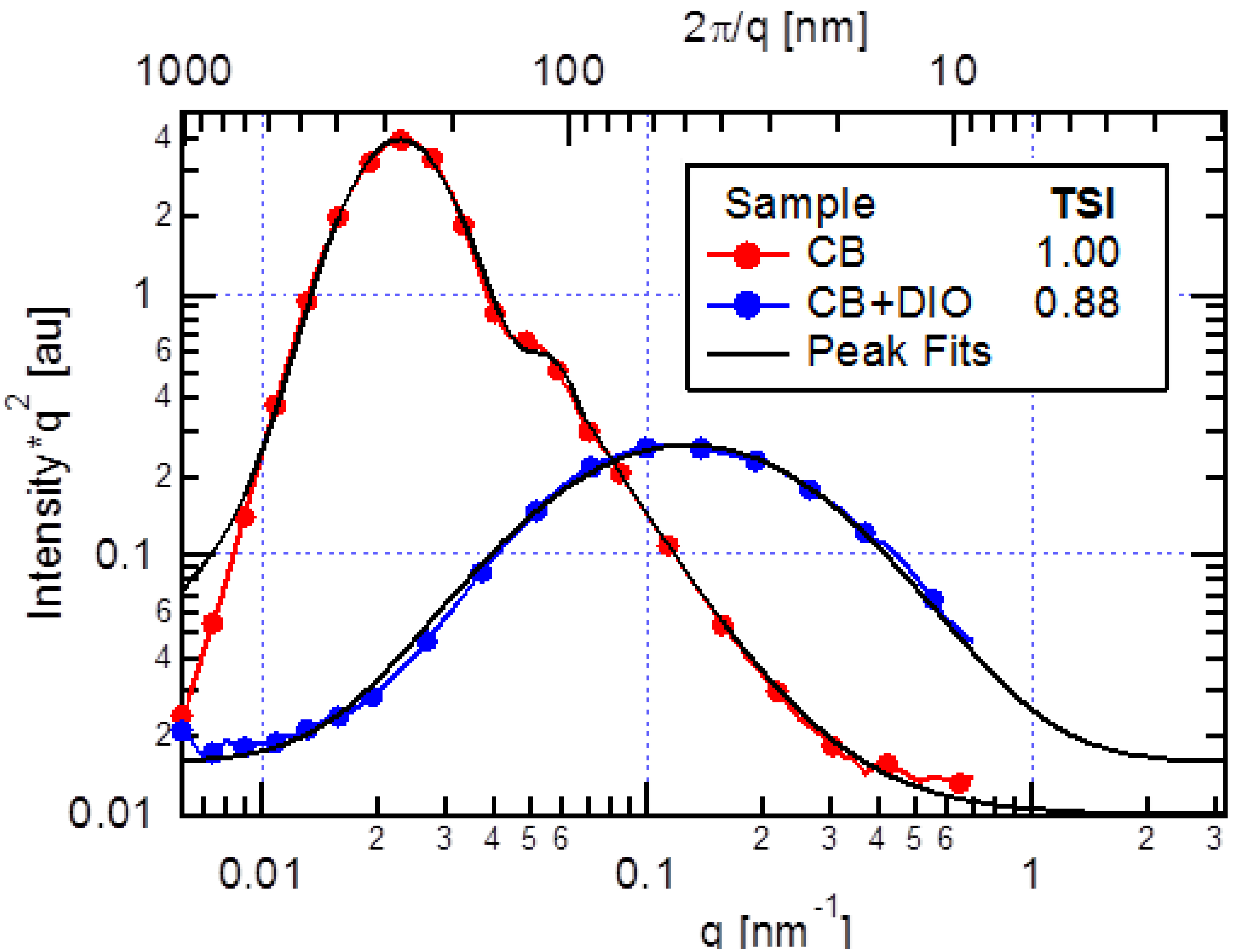


Collins et al. *Adv. Energy Mater.* **3** 65 - 74**,** (2013)

STXM → R-SoXS







Collins et al. *Adv. Energy Mater.* **3** 65 - 74, (2013)

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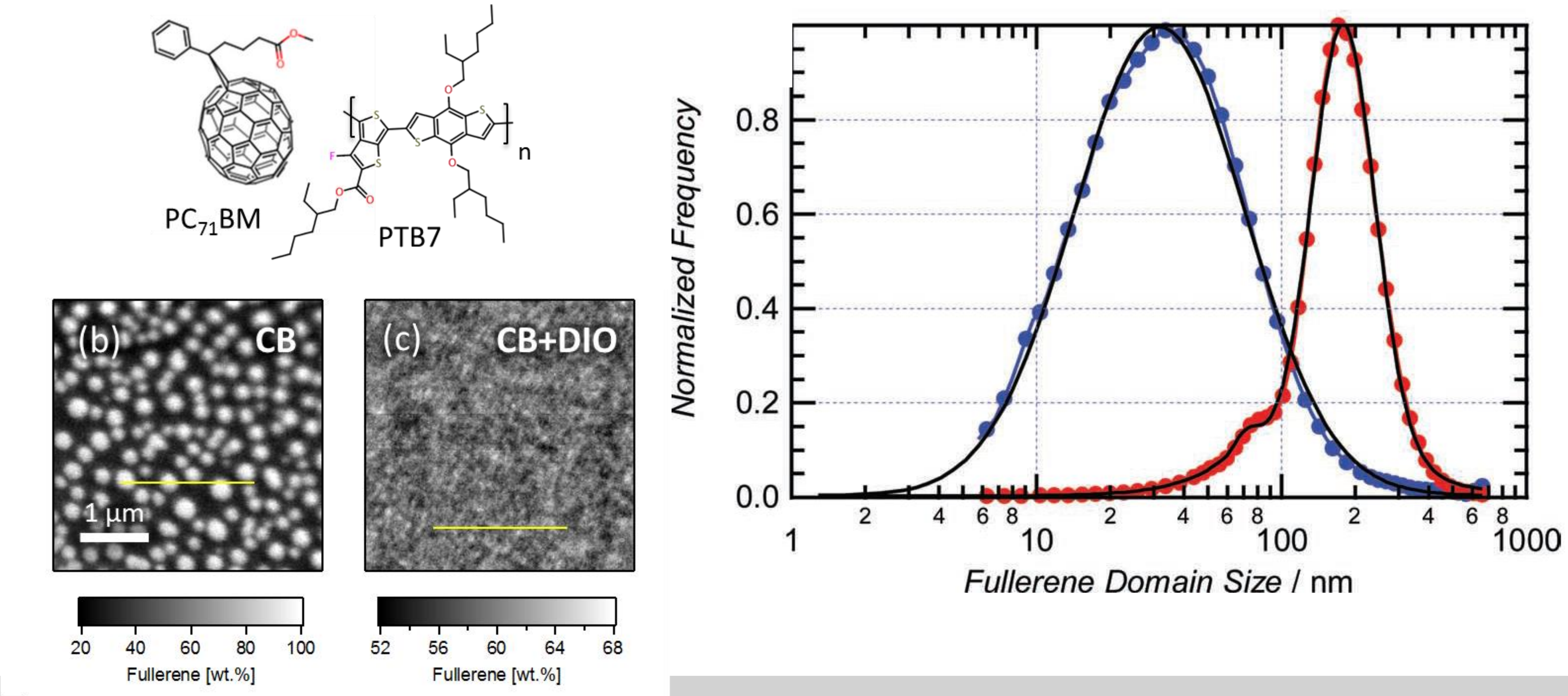
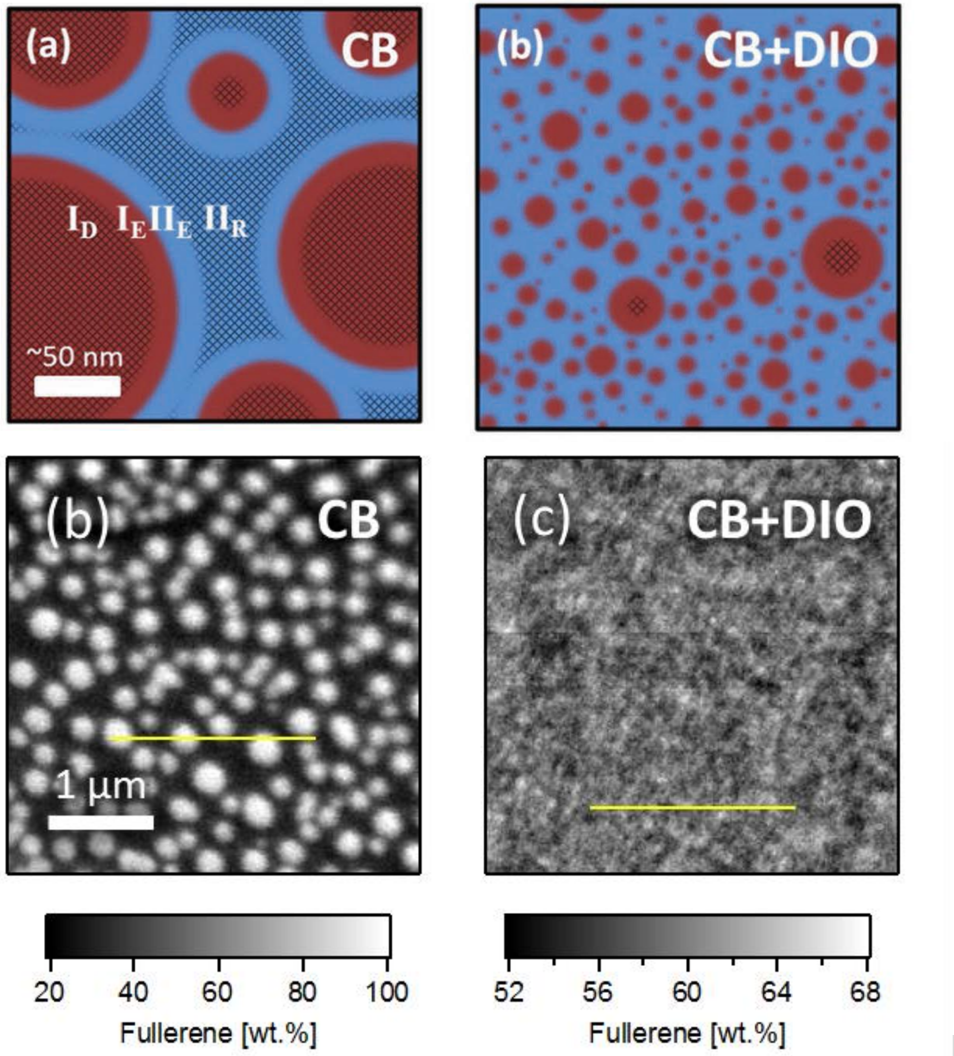
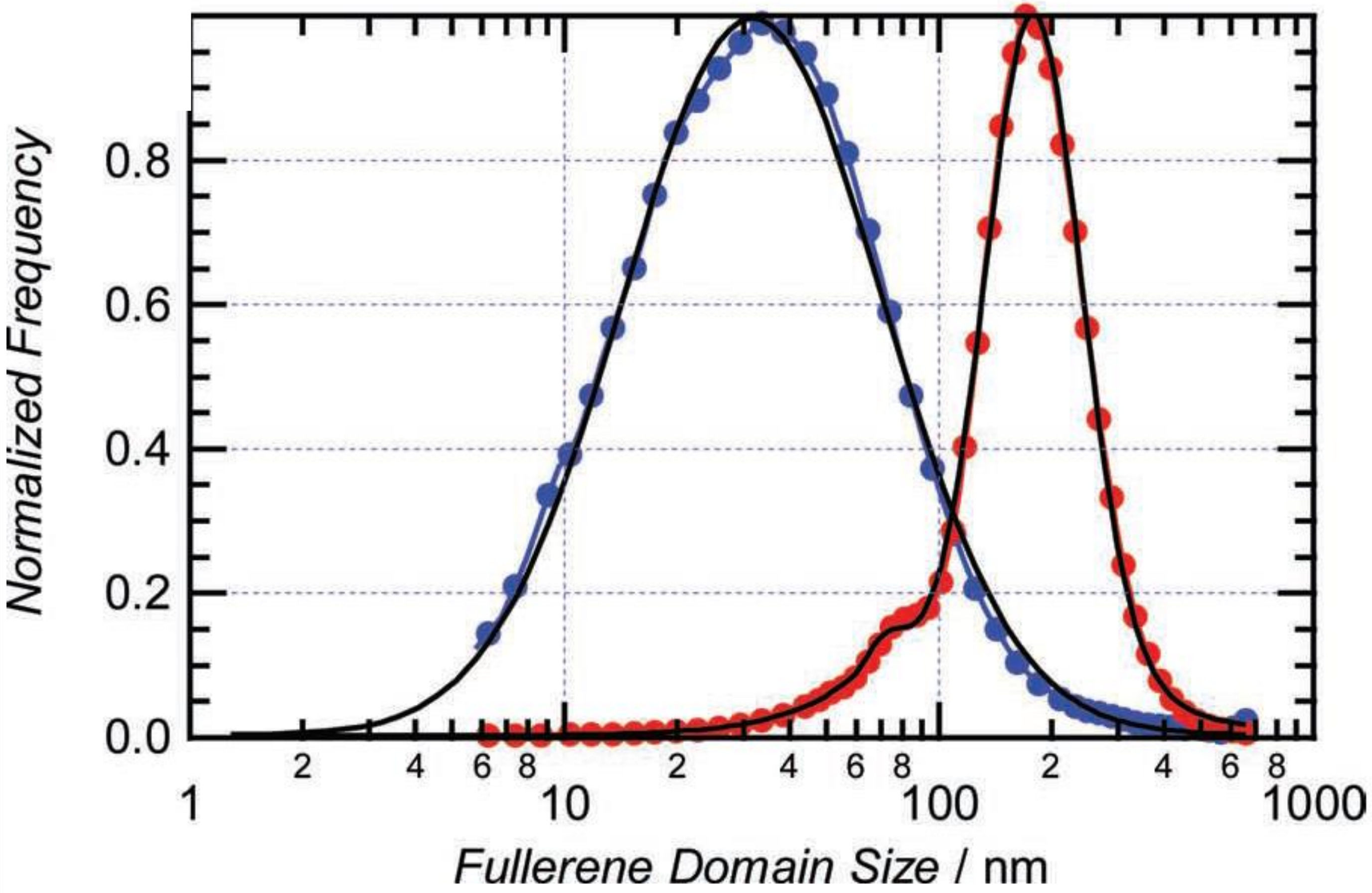
STXM → R-SoXS



Collins et al. *Adv. Energy Mater.* **3** 65 - 74, (2013)

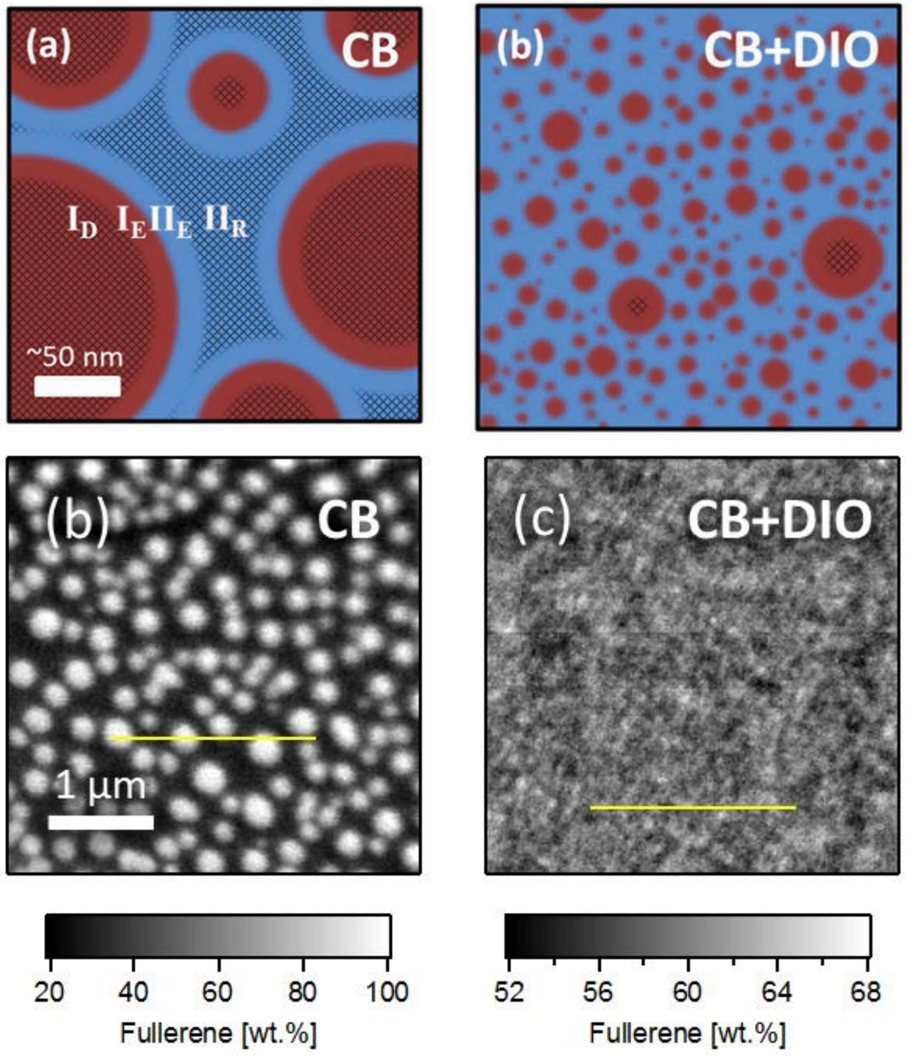
STXM → R-SoXS

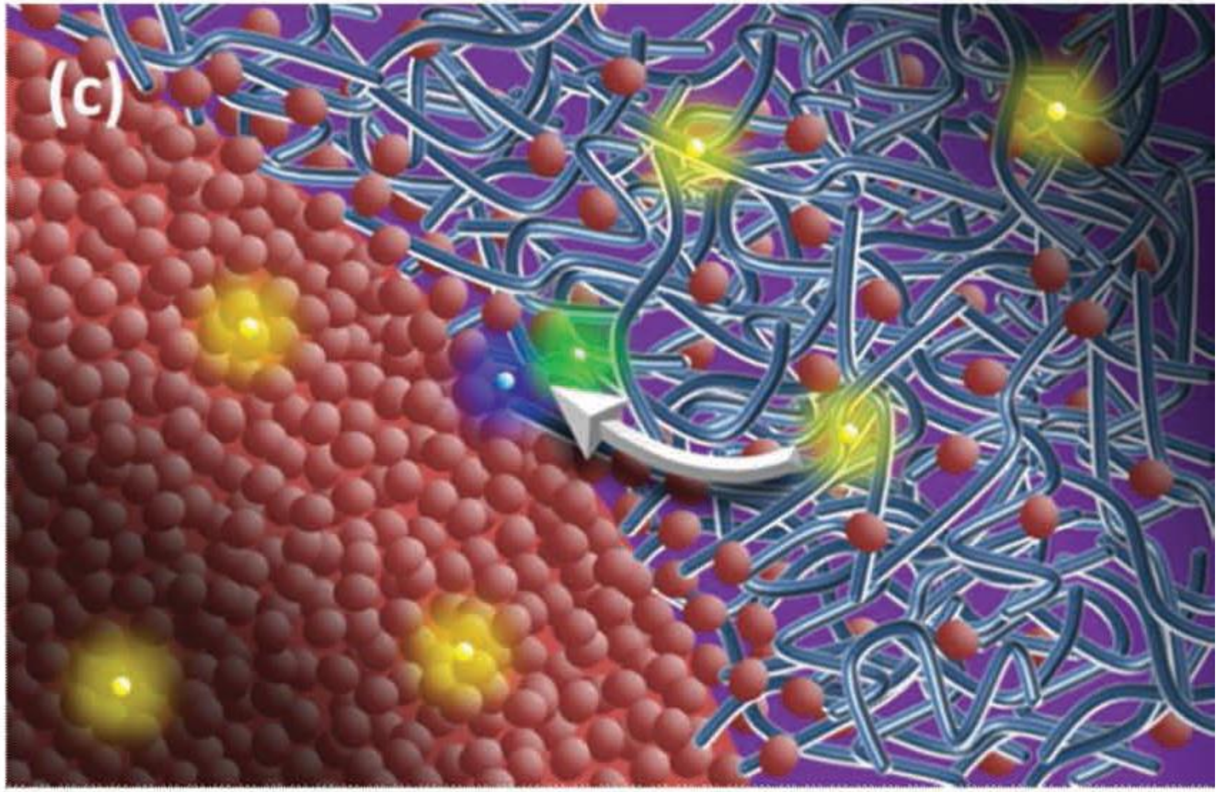




Collins et al. *Adv. Energy Mater.* **3** 65 - 74**,** (2013)

STXM → R-SoXS





Collins et al. *Adv. Energy Mater.* **3** 65 - 74, (2013)

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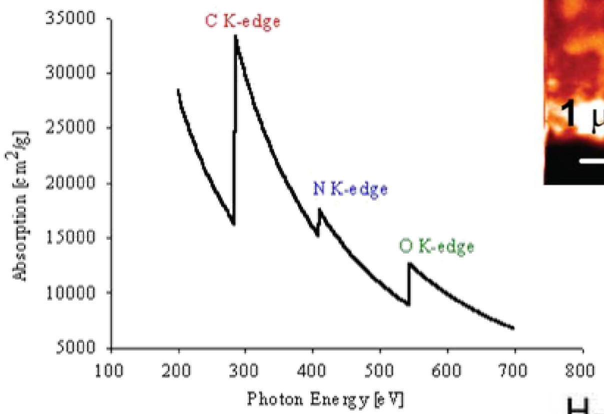
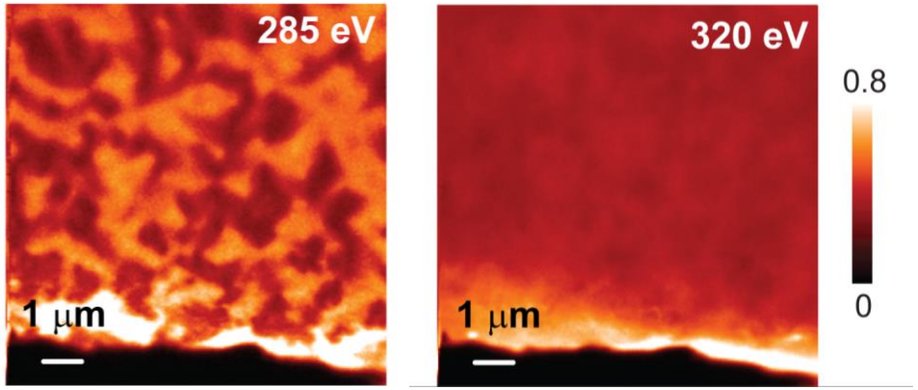
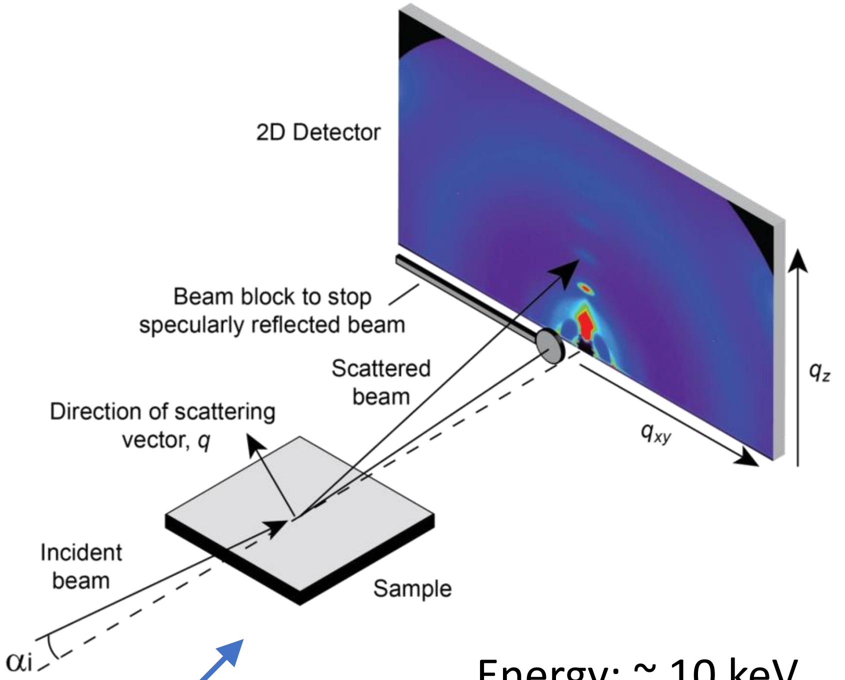
X-rays



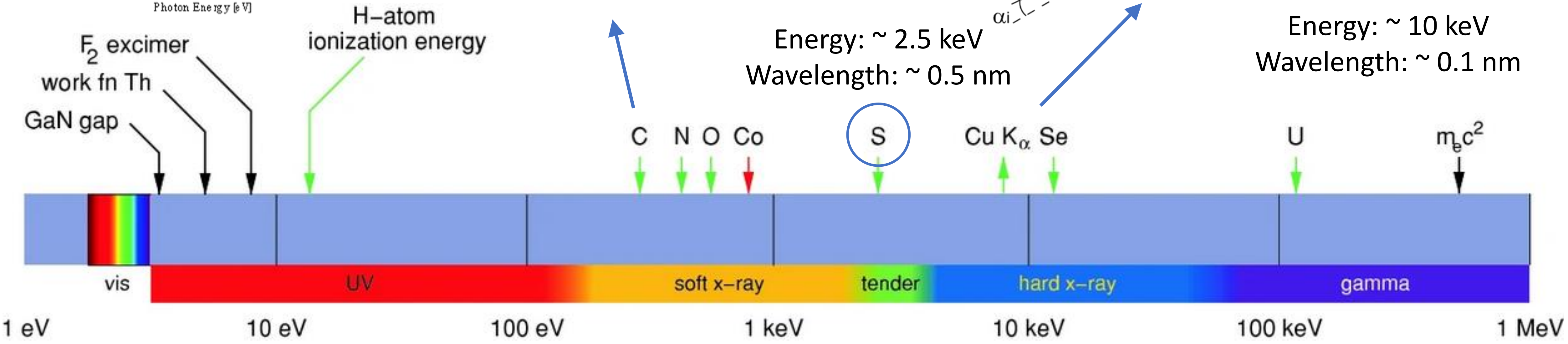




Energy: ~ 285 eV
Wavelength: ~ 4 nm

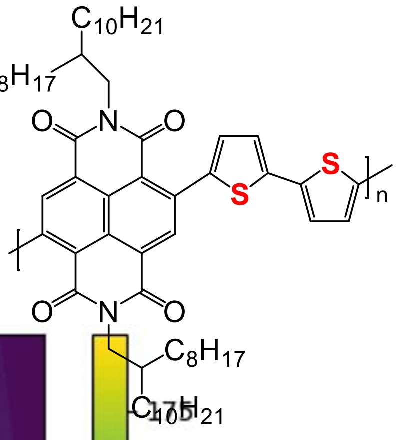
Energy: ~ 2.5 keV
Wavelength: ~ 0.5 nm

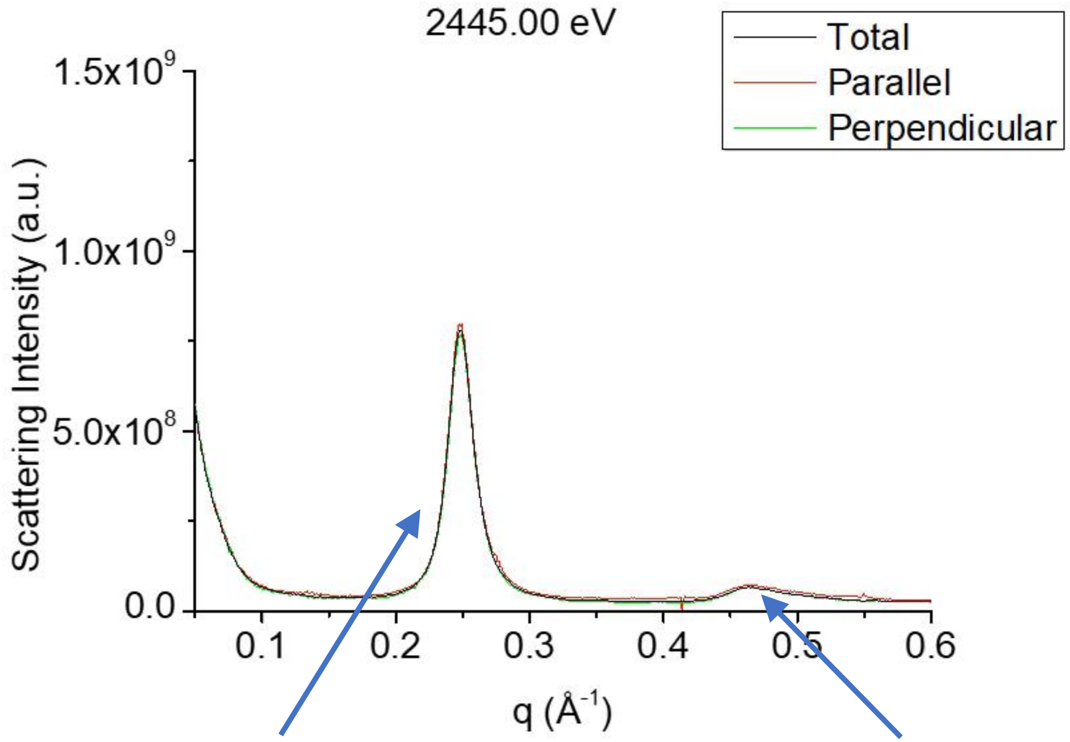
Energy: ~ 10 keV
Wavelength: ~ 0.1 nm



https://doi.org/10.1007/978-3-030-64623-3_1

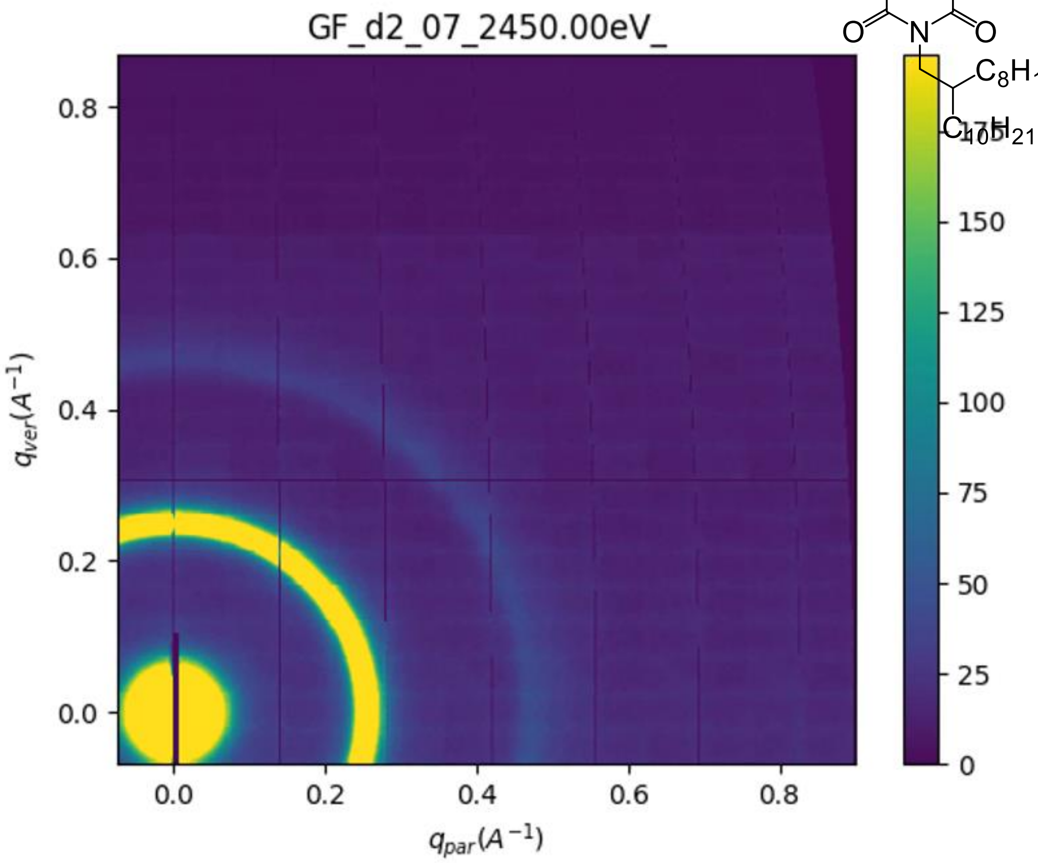
Resonant Tender X-ray Diffraction





(100)

(001)/(200)



X-ray polarisation

Freychet, et al., *J. Am. Chem. Soc.* **143**, 1409 (2021).

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Conclusions

- Organic solar cells are of interest for low-cost, flexible solar panels.
- Efficiency of organic solar cells depends critically on the internal nanostructure of the bulk-heterojunction blends.
- Synchrotron techniques have enabled strong chemical contrast between the donor and acceptor components enabling the nanostructure of bulk heterojunction blends to be studied.
- The ability to tune the X-ray wavelength at synchrotrons allows for unique resonant experiments to be performed.

Acknowledgements