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Monochromated Electron Energy-Loss Spectroscopy of Organic Photovoltaics

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Monochromated electron energy-loss spectroscopy (EELS) is opening up new opportunities for the study of the electronic structure in complex materials. The prospect of mapping band structure with high spatial **and** energy resolution is an exciting prospect. A particularly challenging task is to realise this in organic materials such as polymer matrix composites, biomaterials and organic electronic materials. For example, the processes that generate current in organic photovoltaics (OPVs) are highly dependent on the micro- and nano-structure of the devices, especially at the donor-acceptor (D-A) interface. Hence, the structure of this interface is vital to understanding the efficiency of devices, as this knowledge will provide a foundation for the engineering of new OPV devices with improved power conversion efficiency. Scanning transmission electron microscopy (STEM) EELS can be used to probe the nature and structure of interfaces in OPV devices because it is possible to obtain high energy resolution measurements over large ranges of energy-loss (ΔE).

Due to the beam sensitivity of these materials we are interested in the low-loss spectrum ($\Delta E < 50$ eV) which can be used to determine the complex dielectric function of an OPV material with high spatial resolution over a spectral range that includes the energy range corresponding to the solar spectrum. The complex dielectric function can be used to identify the single electron transitions and collective excitations that occur in OPV materials in the solar energy range. Spatial mapping of the single electron transitions can provide insight about the chemistry and bonding in the vicinity of the D-A interfaces in OPV materials.

Our approach has been to make benchmark measurements of the complex dielectric function for several of the organic materials commonly used in the OPV devices in order to develop a set of organic standards. These materials include copper phthalocyanine (CuPc), fullerene (C_{60}), poly (3-hexylthiophene) (P3HT), and [6,6] phenyl C_{61} butyric acid methyl ester (PCBM). To date we have measured low loss spectra of these materials at 60 kV using a monochromated beam in an FEI Titan[3] 60-300 Image-Corrected S/TEM with typical energy resolutions of 150-200 meV. An example of a low loss EELS spectrum and the imaginary part of the complex dielectric function derived from the spectrum are shown in Figure 1.

Ultimately, these data will be used as standards for EELS measurements made at the donor-acceptor interfaces of actual OPV devices (for instance, the interface in CuPc/C_{60} heterojunction or the interface in a blend of P3HT:PCBM), so that we can measure the signal at the donor/acceptor interface and determine whether or not its signal is simply a linear combination of the two components or if it is more complex. Using this knowledge, we can then begin to determine how the interface relates to the efficiency of the device in order to develop more efficient organic photovoltaics.

References

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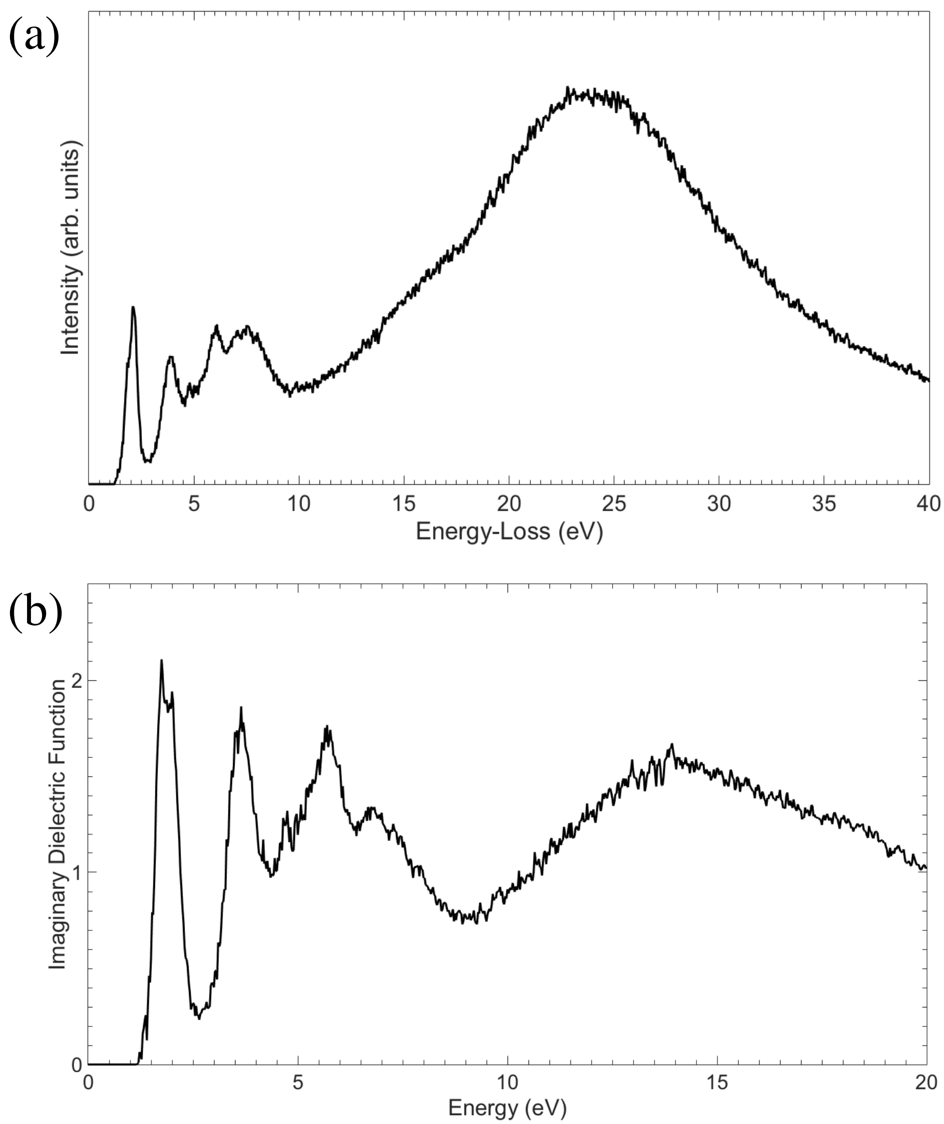

Figure 1: (a) Valence-loss spectrum collected for copper phthalocyanine (CuPc) recorded using 100meV energy resolution. (b) The imaginary dielectric function of CuPc derived from (a) after zero loss peak fitting, deconvolution of plural scattering, and Kramers-Kronig analysis. The peaks in the <5eV energy range can be assigned to single electron excitations between the valence and conduction band.

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