The PHaSE Photovoltaic & Optical Spectroscopy Facility

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The central facilities of the DOE-supported Energy Frontier Research Center “Polymer-Based Materials for Harvesting Solar Energy” (PHaSE) are housed in 1305 sq ft of newly renovated space, Rooms B523 and B524 of the Silvio O. Conte National Center for Polymer Research. The renovation was carried out with EFRC PHaSE ARRA funding. These facilities provide the PHaSE members and external users with a full line of instrument for fabrication of organic solar cells as well as enable characterization of such devices’ performance in the inert gas environment. Additionally, the center is equipped with several experimental techniques for fundamental studies of structural, optical and electronic properties of photovoltaic materials, model systems and devices. This facility centralizes instrumentation, and was designed to be a “user-friendly” facility, allowing easy movement from one research station to another in a natural progression for the characterization of materials and fabrication of devices used for OPV applications.

The following instruments, acquired with EFRC funding, are available in the Facility for characterizing fundamental electrochemical, optical, electronic structure and charge transport properties of materials.

- **UV-VIS-NIR Spectrophotometer** (Shimadzu, UV-3600) for solutions and thin-film samples over 185–3300 nm. TCC-240A thermo-electrically temperature-controlled cell holder with temperature control from 7–60 °C. Specular reflectance and a Praying-Mantis™ diffuse reflectance accessory to study powders, rough-surface solid samples, and high scattering solutions.

- **Photoluminescence Instrument** (Photon Technology International) has an “open architecture” design configured to include PTI’s QuantaMaster™ Spectrofluorometer and TimeMaster™ Lifetime Fluorometer for measuring steady-state fluorescence and phosphorescence as well as fluorescence and phosphorescence lifetimes from 400 ns to 400 ms.

- **Electron Spectroscopy for Chemical Analysis Instrument** (Omicron Nanotechnology, ESCA+S) is a UHV-based, multi-technique platform for surface analysis of materials in Ultraviolet Photoelectron Spectroscopy configuration, analyzing kinetic/binding energies of electrons emitted from material surfaces under UV photo-excitation (He I line, 21.2 eV). The instrument is equipped with an Ar⁺ sputtering gun and state-of-the-art Zalar™ for depth profiling.

- **Epsilon Electrochemical Workstation** (BASi Epsilon Basic) - for Cyclic Voltammetry, Linear Sweep Voltammetry, Chronoamperometry/Chronocoulometry, Controlled Potential Electrolysis, DC Potential Amperometry, Chronopotentiometry, Open Circuit Potential vs. Time methods in pulse, square wave, and stripping modes. This provides the most common methods needed for electrochemical analysis of new solution and film redox systems.

- **Time-of-Flight custom-configured instrument and workstation** – provides measurements of electron and hole mobilities in materials with low intrinsic charge carrier density. The instrument is equipped with an INSTEC HSC302 hot-stage and mK1000 temperature controller for temperature-dependent measurements of mobilities over 20–400 °C.
The following equipment is utilized for steps in the fabrication of photovoltaic devices fabrication that can be done outside of the glove box system (see below), in nearby workstations.

- **UV/Ozone Cleaner** (Jelight Company Inc., UVO Cleaner) - used to remove organic contaminants on surfaces, including substrates used for organic solar cell fabrication.

- **Spin-coater** (Specialty Coating Systems, Spincoat G3P-8) – a compact instrument with user-friendly settings and available multiple operation steps, with each step being repeatable and settable to 0.1 sec, to help varying deposition conditions for optimizing film morphology.

- **Precision Hot Plate** (Electronic Microsystems LTD, model 1000-1) – for the thermal annealing of films from 50–150 °C with an accuracy to ±1% across the working surface.

- **Surface Profiler** (KLA Tencor, Alpha-Step IQ) is a computerized, high-sensitivity stylus-based instrument that measures micro-roughness to at least 1 Å over short distances, and waviness in a scan over a full surface length of 10 mm, plus step-height in various applications.

- **Laboratory Vacuum Oven** (Lindberg/Blue M, VO914SA-1) – designed for drying, curing, outgassing, aging, process control and other applications which require elevated temperature in reduced atmospheres or vacuum/purge with non-flammable and inert atmospheres.

- **Polisher/Grinder** (Struers, TegraPol-31 with TegraForce-3) – grinding and polishing machine for specimens of up to 300 mm disc diameter.

- **Vacuum Evaporator** (Thermionics Laboratory, VP-90) – for metal film (electrode) deposition.

- **Additional device fabrication steps** are typically done inside our custom-designed, two-compartment glove box system (MBraun) in a moisture and oxygen free non-reactive atmosphere (<1 ppm). The following devices are located inside of the glove box system.

- **Spin-coater** (Specialty Coating Systems, Spincoat G3P-8) – for spin-coating of active layers.

- **Precision Hot Plate** (Electronic Microsystems LTD, model 1000-1) – for pre-annealing of active layers and post-annealing of photovoltaic devices.

- **Two-Source Thermal Evaporator** (MBraun) and E-beam Evaporator (MDC vacuum products) – for metal and metal oxide film deposition.

For the photovoltaic device performance characterization, the following equipment is available inside the glove box’s device characterization compartment. The main glove box pre-dated the startup of PHaSE, but PHaSE funding has allowed updates, maintenance, and addition of some ancillary features.

- **300W Solar Simulator** (Newport/Oriel Instrument, 91160) with AM1.5G spectral correction filter produces a uniform, collimated, 2 × 2 inch output with close spectral match to sunlight at a power equivalent to up to ~2 Suns. A KG5-filtered Silicon reference cell (Newport/Oriel, 91150V) is used for the irradiance calibration. I-V characteristics of solar cells under standard illumination conditions are measured using a Keithley 2400 Source Meter.

- **The QE-PV-SI Measurement Kit** (Newport/Oriel Instruments) with 150 W Xe arc lamp, monochromator and calibrated silicon reference cell with power meter, is used for Quantum efficiency (QE)/Incident Photon to Charge Carrier Efficiency (IPCE) measurement for solar cells over a 350–1100 nm spectral range in dc and ac modes, allowing the testing of photovoltaic devices with long photo-response times or low power conversion efficiencies, respectively.

**Other Instrumentation at UMass Amherst:** Although routine research space and equipment used by individual investigators to pursue PHaSE funded work are not listed, several capabilities have been augmented and supported by PHaSE to promote team collaborations or faster synthetic and analytical
throughput. The Facility Director does not oversee these but they are available by collaborative arrangement with the PHaSE investigator whose group oversees the instrument and keeps the co-Directors informed of maintenance needs. These instruments include a crystal deposition and transport measurement facility (Briseno), Fourier Transform Infrared (FTIR) Spectrometer (Lahti), Teledyne ISCO CombiFlash Rf-200 UV-Vis Automated Flash Chromatography System, (Lahti), Milestone START Microwave Reactor System (Venkataraman), Optical AFM spectroscopy laboratory (Barnes). NSOM (Barnes), Time-resolved photoluminescence (PL) lab station, PicoQuant pulsed diode lasers. Sample PL is spectrally dispersed with a monochromator, detected with a cooled multichannel plate photomultiplier tube (Hamamatsu R3809U-51) or avalanche photodiode (Id Quantique 100-APD), and analyzed with a TCSPC system (Becker-Hickl SPC-630 or PicoQuant PicoHarp 300). The laser and detection systems typically provide a 70 ps time resolution for PL measurements (Barnes). For computation, an Intel QuadCore i7 Lintel computer workstation with openSuSe O/S and the following software for computational modeling: Spartan 2010 (Wavefunction), Gaussian 09, GAMESS (Lahti).

Other facilities available at Amherst: The EFRC benefits from the Shared Experimental Facilities for the characterization of polymeric materials, maintained by the NSF-supported Materials Research Science and Engineering Center. These include: Molecular Weight Determination, X-Ray Scattering, Thermal Characterization, the Keck Nanostructures Laboratory, Optical Microscopy, NMR, the Keck Electron Microscopy Facility, Computing, Rheology, Spectroscopy and Surface Science. All are essential for the Center’s research. Center investigators have also used the Materials Research Facilities Network to perform dynamic secondary ion mass spectroscopy experiments at the University of California at Santa Barbara. The Center also benefits will from the Shared Experimental Facilities of the NSF-supported Center for Hierarchal Manufacturing (CHM), which maintains clean room facilities, as well as facilities for the fabrication and characterization of nanostructured materials. These Shared Experimental Facilities have technical support staff (seven at the Ph.D. level) provided by the University of Massachusetts Amherst, and the Commonwealth of Massachusetts provides partial support for equipment maintenance.