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DOE Energy Frontier Research Center for Achieving Stability in Organic and Perovskite Energy Materials & Structures

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Energy Frontier Research Center for Achieving Stability in Organic and Perovskite Energy Materials and Structures

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Poor stability of organic solar cells impedes their commercial application, despite their high efficiency. Similar degradation processes also affect blue and white organic light emitting diode materials and structures at high brightness, particularly those that are solution processed. Yet, these organic energy materials and structures have enormous potential, leading BES to identify the basic science underlying their degradation to be of *paramount importance*; dramatic developments in perovskite photovoltaics accentuate this issue. The objective of this EFRC is to systematically investigate the fundamental mechanisms underlying stability and degradation in organic, hybrid, and perovskite photovoltaic (PV) and solid state lighting materials and structures. The Center will additionally focus on processes at organic/organic (O/O) and organic/inorganic (O/I) interfaces far from equilibrium at the atomic and electron level, thereby addressing one of the Grand Challenges in materials studies. Activities will include modeling, synthesis, and characterization over a wide range of time scales, and will focus on the effects of processing and fabrication. The Center's specific goals are to investigate:

- Inherent degradation processes, as found in small molecules, polymers, and the new highly-efficient perovskite PV materials and structures, as well as the new thermally-activated delayed fluorescence materials and structures. Instability in these materials and at the O/O and O/I interfaces must be overcome to realize their potential in PV and lighting structures.
- Deposition and fabrication conditions that affect stability, in particular mechanisms differently affecting solution-processed vs. thermal vacuum evaporated films/structures, and the role of defects, impurities, UV irradiation, temperature, oxygen, and humidity.
- Optimum thermal management, and how it differs for solar and high brightness lighting structures.

These diverse questions will be addressed using a comprehensive center approach based on expertise in theoretical studies, synthesis, fabrication, and characterization (e.g., structural, transient photocurrent, ultrafast ultrabroadband, microwave, and magnetic resonance). The work will elucidate degradation mechanisms in materials far from equilibrium to study complex structures at organic interfaces, and spectroscopies will probe electron and molecular dynamics down to the fs time scale. Predictive density functional theory and molecular dynamics modeling will guide the synthesis and characterization of novel materials for high-efficiency stable PVs, particularly low-gap polymers and perovskites. Characterization will occur at various stages of degradation induced by light, bias, and/or environment; also, mesoscale structures and novel nanoparticles will be embedded to study their effects on stability and degradation. The Center's scientific outcomes will enable the achievement of efficient and <u>*stable*</u> structures for harvesting solar energy, as well as stable lighting products that save up to 50% over current electricity levels. These advances will impact the application of generalized stability schemes to other functional organic molecules used in energy technologies.