NREL Highlights SCIENCE

# 200% Efficient Singlet Fission Observed

NREL scientists confirm the first molecular compound designed specifically to exhibit exciton multiplication.

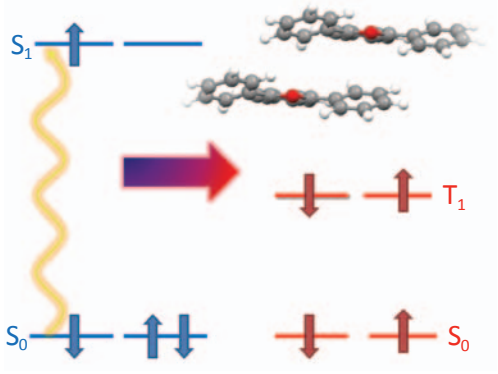
Singlet fission is the molecular analog of Multiple Exciton Generation (MEG) in inorganic quantum dots. It creates two triplet states from an excited singlet state and potentially produces two electron-hole pairs per absorbed photon in a solar cell, increasing the energy conversion efficiency. In a Basic Energy Sciences (BES) Program-sponsored collaboration with Professor Josef Michl at the University of Colorado, NREL researchers spectroscopically observed a 200 ± 30% triplet quantum yield in a thin film of the compound 1,3-diphenylisobenzofuran (DPIBF), confirming theoretical work by Professor Michl on molecules designed with specific properties favorable for singlet fission.

The stacking arrangement of molecules and the appropriate singlet and triplet state energy level alignment led to the high efficiency. Prior attempts that arranged DPIBF molecules in other geometries led to a yield of only a few percent. Thermodynamic modeling indicates a simple multi-layer solar cell based on singlet fission could increase the photoconversion yield by more than one third.

The Hydrogen Fuel Initiative within the U.S. Department of Energy's Office of Science, BES Program, Division of Chemical Sciences, Biosciences, and Geosciences sponsored this research.

**Technical Contact:** Justin Johnson, *justin.johnson@nrel.gov*

**References:** Johnson, J.C.; Nozik, A.J.; Michl, J.; 2010. *J. Amer. Chem. Soc.*, 132, 16301.




## Key Research Results

### Achievement

Singlet fission is the molecular analog of Multiple Exciton Generation (MEG) that NREL has been working on in quantum dots for the last several years, including our Energy Frontier Research Center (EFRC) co-led with the Los Alamos National Laboratory. This work is also a key part of NREL's Hydrogen Fuel Initiative Renewal proposal currently under review by BES Chemistry.

### Key Result

NREL researchers observed a 200 ± 30% triplet quantum yield in a thin film of the compound 1,3-diphenylisobenzofuran (DPIBF), confirming theoretical work on molecules designed with specific properties favorable for singlet fission.

### Potential Impact

Thermodynamic modeling indicates a simple multi-layer solar cell based on singlet fission could increase the photoconversion yield by more than one third.

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

1617 Cole Boulevard | Golden, Colorado 80401-3305 | 303-275-3000 | www.nrel.gov

**NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.**

NREL/FS-5900-51751 • June 2011