

## Keynote speech

# Novel Organic Materials for Photovoltaic Devices

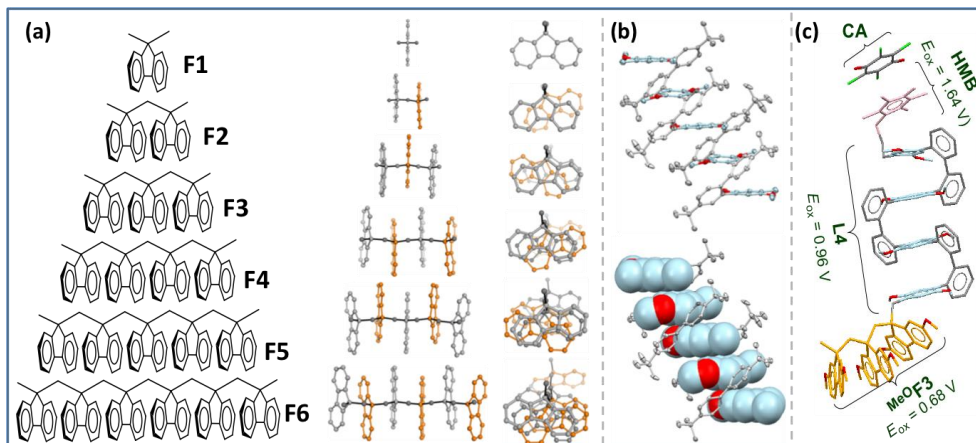
Professor Rajendra (Raj) Rathore

*Department of Chemistry, Marquette University, Milwaukee, Wisconsin, USA*

Current climate changes have caught no one by surprise as today's economic growth from which we all benefitted, albeit to a different extent, came from excessive usage of fossil fuels –a major source of global warming. Despite the deniability by many world leaders, if the CO<sub>2</sub> emission -- the main culprit of global warming -- is not checked, the Earth as we know will cease to exist. The increasing energy needs of today must be met from alternative sources rather than burning of limited fossil fuels. Unlimited and free solar energy has presented itself as the ultimate environmentally-friendly alternative. This talk will address our efforts to generate fundamental knowledge to advance the functioning and efficiency of modern photovoltaic devices for solar energy harvesting and storage.

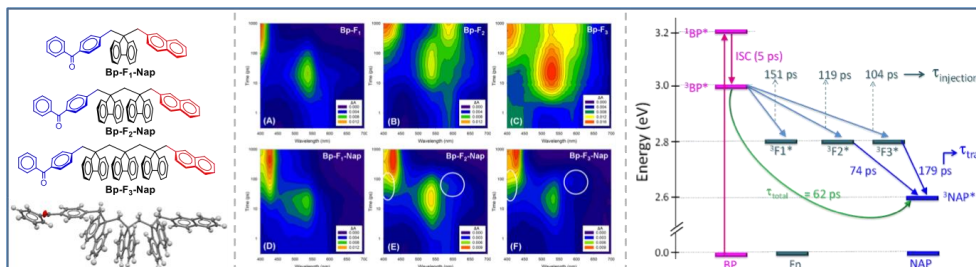
The general objective of our research efforts is to design and synthesize electroactive molecules for application in organic electronic and photovoltaic devices, which convert light energy into electrical energy. Compared to current inorganic devices, which often rely on expensive and rare inorganic materials, organic-based electronics offer significant advantages in terms of cost and scalability, their full potential is yet to be utilized.

Our approach has used cofacially-arrayed DNA-like electro-active organic molecules (see representative structures below), and much of our current research efforts focus on the structure-function relationship of these materials. In this work, we exploit a variety of techniques such as electrochemistry, X-ray crystallography, and various electronic and emission spectroscopic methods including time-resolved transient laser spectroscopy on the millisecond to femtosecond timescale. The design, synthesis and study of novel polychromophoric molecules that can be readily prepared by versatile synthetic routes provide the foundation for the discovery of new materials for long-range charge transport and hence practical applications in modern photovoltaic devices.

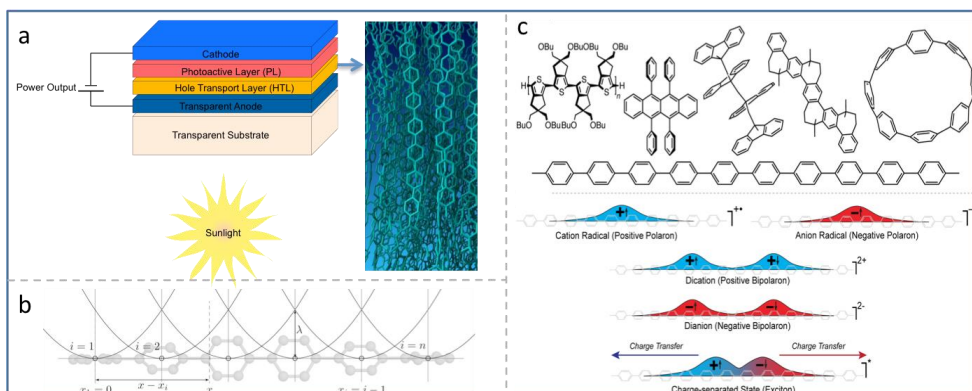


Two representative current research activities will be highlighted in this presentation:

Using a series of [D-molecular wire-A] systems, where D is a energy donor, A is a energy acceptor, and stacked polyfluorenes are molecular wires(see below), we demonstrated sequential energy transport from D to A through DNA-like molecular wires. The ultrafast laser spectroscopic measurements demonstrated that a crossover occurs between single step tunneling and multi-step hopping for energy transfer as the wire length increases. This change in the mechanism of energy transfer was established by direct spectroscopic observation of the spacer-occupied excited state. The details of this work have been described in a Science article (Science2010, 328, 1547-1550. DOI:10.1126/science.1189354).



Organic electronics and photovoltaics offer the next generation of eco-friendly, flexible, and low-cost electronic devices that can replace and/or complement traditional devices based on inorganic materials. A key research challenge, which needs to be overcome for realizing the vision of organic electronics/photovoltaics as a more innovative, accessible, and sustainable approach to growing our electronic world, is increase of efficiency of organic electronic devices (Figure a, below).



Therefore, a better understanding of the structure-function relationship is required for the design of next-generation advanced materials such as wires, switches, transistors, etc. This undertaking requires developing a detailed understanding of structure-function relationship with the aid of computational chemistry and recently developed theoretical models as tools (Figure b, above). These recently developed tools broadly impact not only the field of photovoltaics but will have direct implications to understanding the chemical reactivity in general (note that mechanisms of many organic reactions involve the formation of cation- or anion-radicals, e.g. Figure c, above) and long-range charge transfers in biological systems.