



Chemistry Department Special e-Seminar

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Rational Molecular Design Enables Efficient Organic Solar Cells and Organic Light Emitting Devices



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Abstract: Conjugated polymers and small molecules have great potential to meet one of the world's most critical challenges, clean energy production, in the following decades. Owing to their semiconducting properties, organic conjugated molecules are promising candidates for clean energy applications such as organic solar cells (OSC) and organic light-emitting diodes (OLED) due to their low-cost, light-weight, flexible. This study covers the rational molecular design for efficient OLEDs and OSCs. The first chapter covers the observation of thermally activated delayed fluorescence (TADF) in conjugated systems. In this study, six different OLEDs were produced using two different anodes (ITO and graphene) and three different emitters (green, blue, and yellowish-green). The maximum external quantum efficiency, EQE is 30.8%, and the maximum lumen is 17007cd.m⁻². The second chapter includes the effect of mono-fluorine substitution of benzothiadiazole and replacing the alkoxy group with alkylthienyl on the performance of bulk-heterojunction (BHJ) OSCs. Among three random polymers, the best performing device exhibits a power conversion efficiency, PCE of 9.21% with a fill factor, FF of 60%, and 15.4 mA.cm⁻² short circuit current density, J_{sc}. In the third part, ternary OSCs will be covered. Optimizations resulted in an OSC with a PCE of 9.26%, a J_{sc} of 19.8 mA cm⁻², and a FF of 60% was produced.

