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# Study Questions for Experiment 8

### About Dye-Sensitized Solar Cells (DSSC)

* How does an oxidized dye molecule get reduced back to its original state?
* What property of the TiO2 nanocrystalline layer allows efficient light absorption?
* What property of the TiO2 nanocrystalline layer allows efficient electron flow?
* Would [Ru(bpy)3]2+, the dye used in Experiment 7, be a good dye for a solar cell? Why or why not?
* What is the function of the I3– in a DSSC?
* What is the function of the I– in a DSSC?
* The counter electrode in a DSSC must be covered with C nanocrystals (soot) or Pt nanocrystals in order to work. What is the function of this layer?
* After an electron is donated from an excited dye to a TiO2 crystal, what process may occur, decreasing the solar cell’s output?
* If we describe a DSSC as a galvanic cell, which chemical species acts as the reductant? As the oxidant?
* If the cathode constantly produces I– and consumes I3–, why doesn’t the solar cell eventually reach equilibrium and stop?

### About Excited States

* In an excited-state dye molecule, which frontier orbital behaves as the reduction orbital, and thus determines the reduction potential?
* In an excited-state dye molecule, which frontier orbital behaves as the oxidation orbital, and thus determines the oxidation potential?
* What two experimental techniques can determine the reduction potential of an *excited-state* molecule?
* When a ruthenium dye is excited by light, does it become a better oxidant or a better reductant.

# Answers

### About Dye-Sensitized Solar Cells (DSSC)

* How does an oxidized dye molecule get reduced back to its original state?
* *It accepts an electron from I– (i.e., is reduced).*
* What property of the TiO2 nanocrystalline layer allows efficient light absorption?
* *This layer has a high surface-area-to-volume ratio, which allows a high concentration of adsorbed dye molecules to intercept the light.*
* What property of the TiO2 nanocrystalline layer allows efficient electron flow?
* *TiO2 is a semiconductor, so it has a moderate conductivity.*
* Would [Ru(bpy)3]2+, used in Experiment 7, be a good dye for a solar cell? Why or why not?
* *This molecule would not bind to TiO2 crystals, and thus would not donate electrons when excited.*
* What is the function of the I3– in a DSSC?
* *I3– accepts electrons from the counter electrode, forming 3I–*
* What is the function of the I– in a DSSC?
* *I– donates electrons to oxidized dye molecules, allowing them to continue absorbing light.*
* The counter electrode in a DSSC must be covered with C nanocrystals (soot) or Pt nanocrystals in order to work. What is the function of this layer?
* *This layer catalyzes the reduction of I3– at the counter electrode, allowing I– to be formed at a reasonable rate to keep the solar cell working.*
* After an electron is donated from an excited dye to a TiO2 crystal, what process may occur, decreasing the solar cell’s output?
* *The electron recombines with the oxidized dye molecule, and contributes no charge to the circuit.*
* If we describe a DSSC as a galvanic cell, which chemical species acts as the reductant? As the oxidant?
* *The excited-state dye molecule is both reductant and oxidant.*
* If the cathode constantly produces I– and consumes I3–, why doesn’t the solar cell eventually reach equilibrium and stop?
* *As I– accumulates, it diffuses to the photoanode and is consumed as it reduces dye molecules. This depletion ensure continued diffusion, so the reaction never stops (as long as light is present and continues to make oxidized dye molecules).*

### About Excited States

* In an excited-state dye molecule, which frontier orbital behaves as the reduction orbital, and thus determines the reduction potential?
* *The LUMO, which contains a single electron, is the reduction orbital.*
* In an excited-state dye molecule, which frontier orbital behaves as the oxidation orbital, and thus determines the oxidation potential?
* *The HOMO, which contains a single hole, is the oxidation orbital.*
* What two experimental techniques can determine the reduction potential of an *excited-state* molecule?
* *Electrochemical voltage measurements and luminescence measurements allow us to estimate the free energy and convert it to a cell potential.*
* When a ruthenium dye is excited by light, does it become a better oxidant or a better reductant?
* *It becomes* ***both*** *a better oxidant* ***and*** *better reductant*.