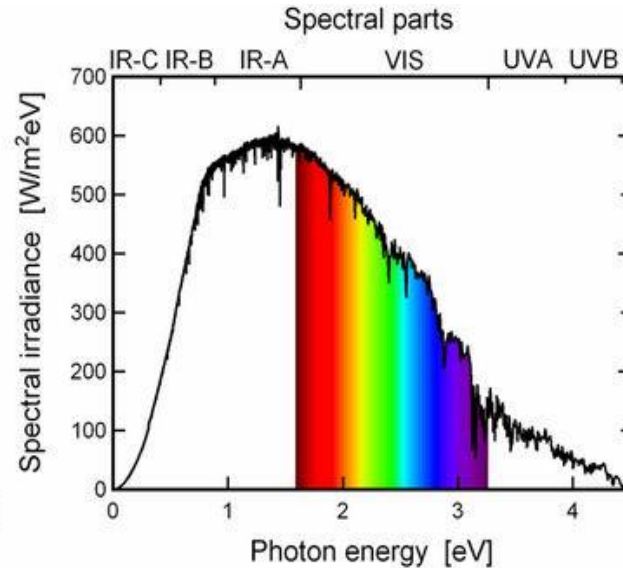
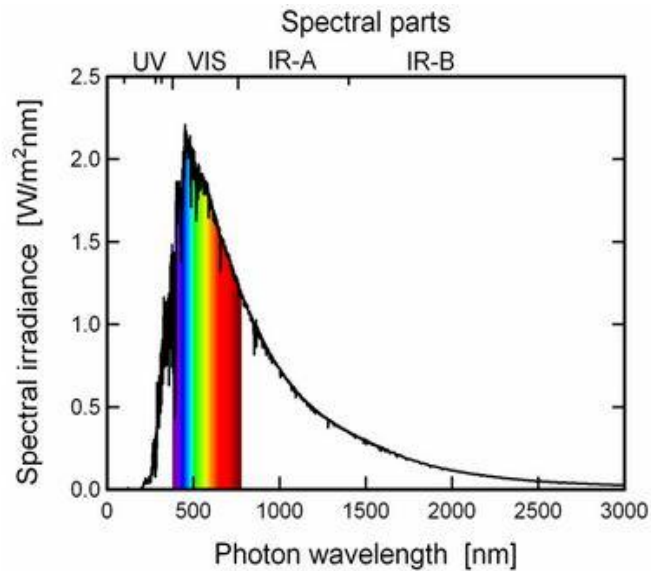
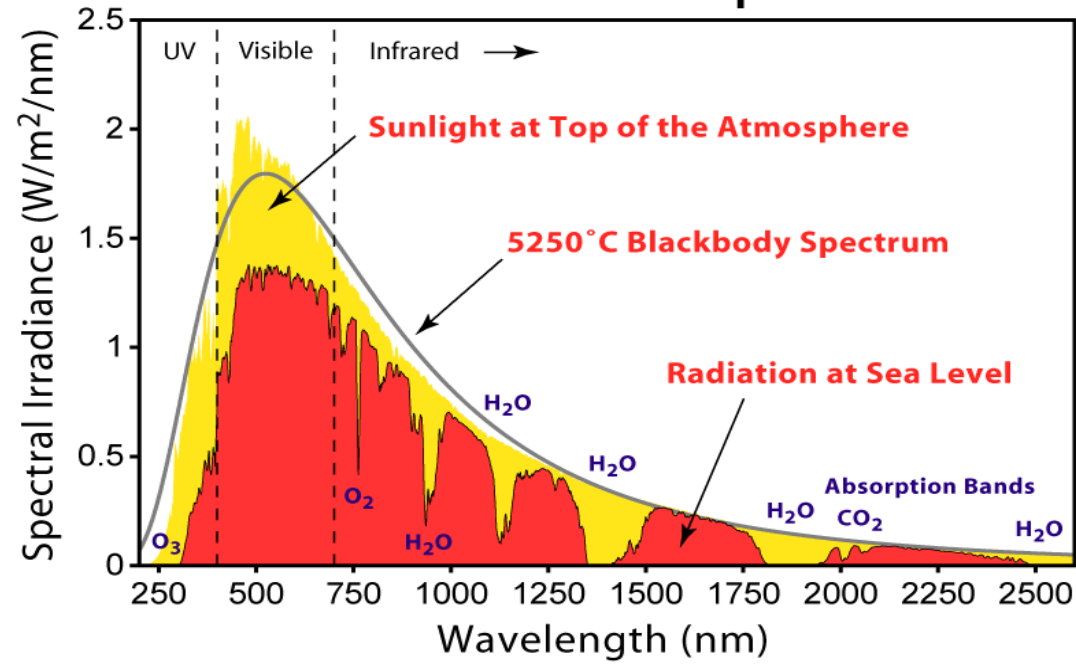


# Solar Radiation Spectrum

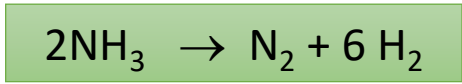


## COMO APROVEITAR A ENERGIA SOLAR???

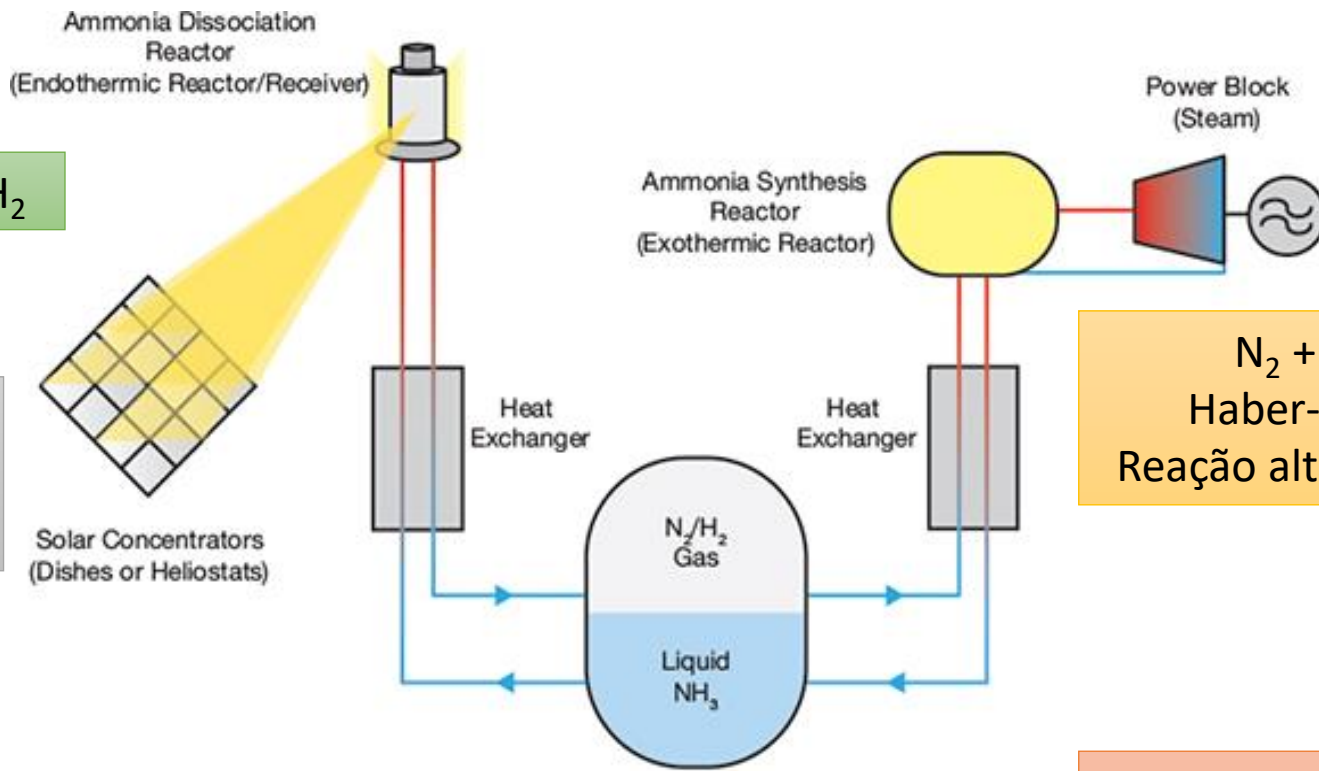
Uso de células fotovoltaicas  
a base de Si



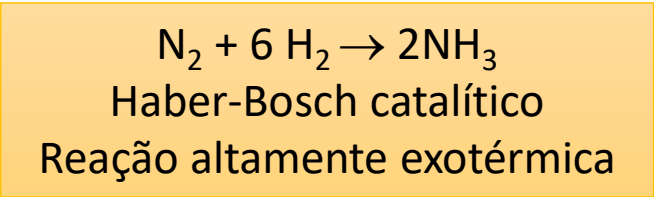
OUTRAS FORMAS DE UTILIZAÇÃO DA ENERGIA SOLAR  
CICLO DA AMÔNIA (NH<sub>3</sub>)  
Ciclo termoquímico catalítico



Espelho parabólico para concentrar a radiação solar



Gerador de trabalho mecânico convertido em elétrico

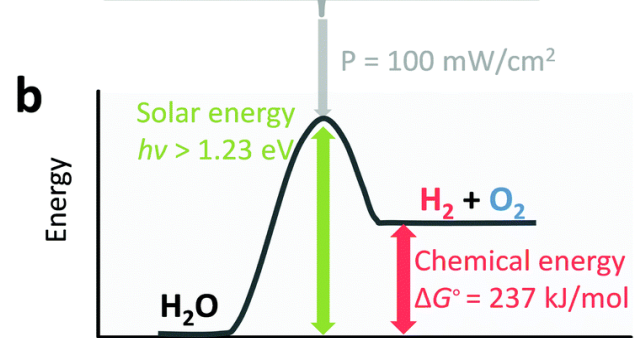
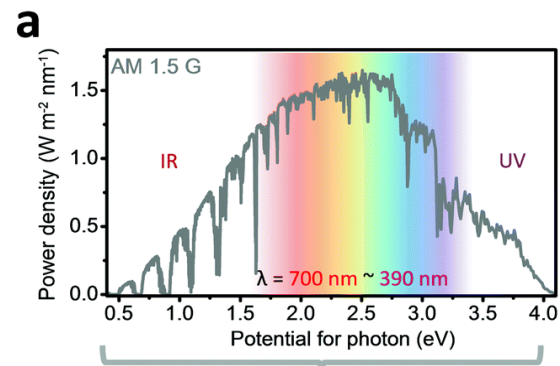


- Storage of Reactants at Ambient Temperature
- High-Pressure Underground Storage of Gases

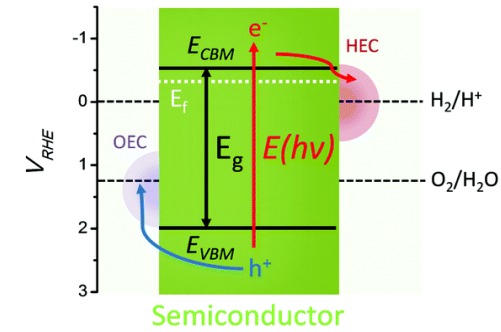
**Problemas:**  
Escape de amônia  
Alta pressão e temperatura  
Escape de hidrogênio  
Geração de óxidos de nitrogênio poluentes

<https://www.iche.org/resources/publications/cep/2017/july/leveraging-ammonia-industry-solar-energy-storage>

**FOTOLETRÓLISE DA ÁGUA  
PARA GERAR HIDROGÊNIO  
USANDO FÓTONS COM ENERGIA  
MAIOR QUE 1,23 eV  
 $h\nu \geq 1,23 \text{ eV}$**



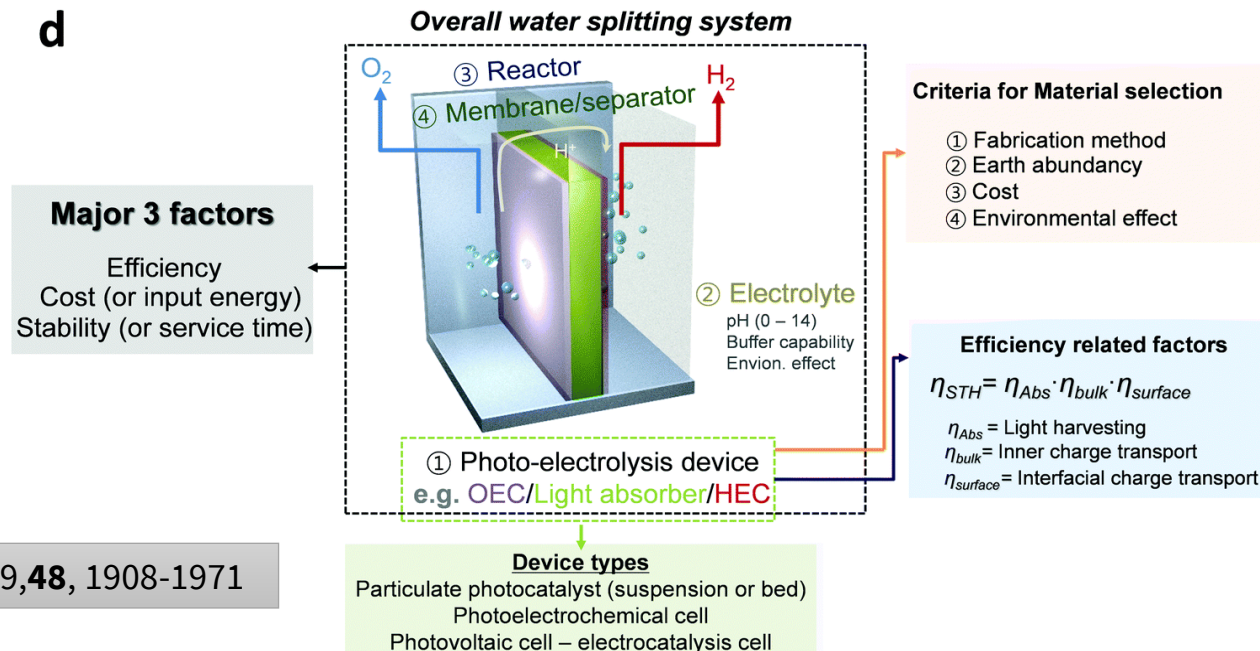
**c** Photon driven-water electrolysis



$$E(h\nu) \geq E_g + \eta_{\text{loss}} > 1.23 \text{ V}$$

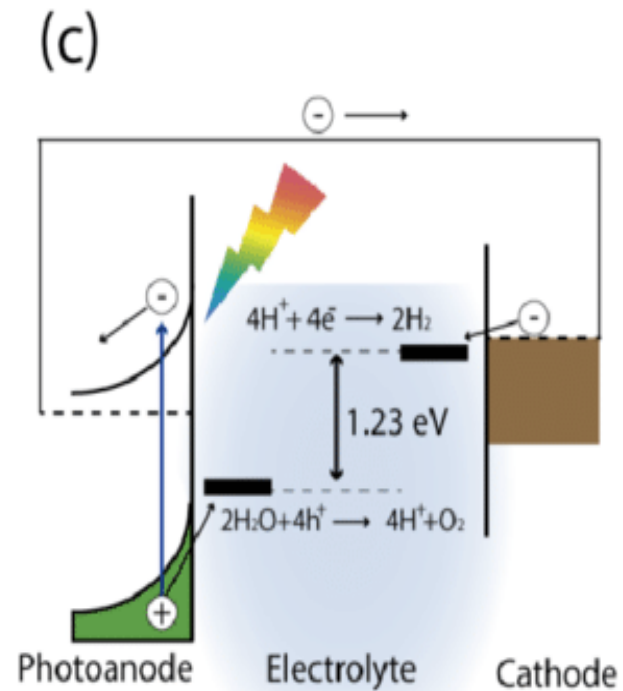
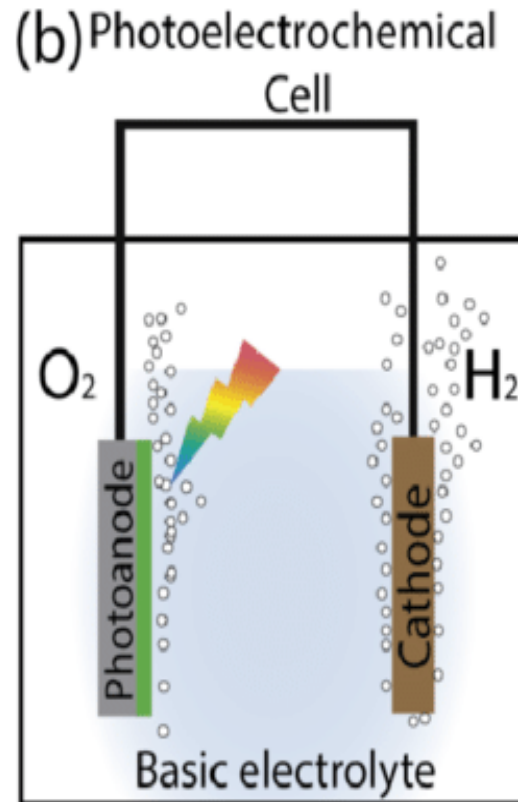
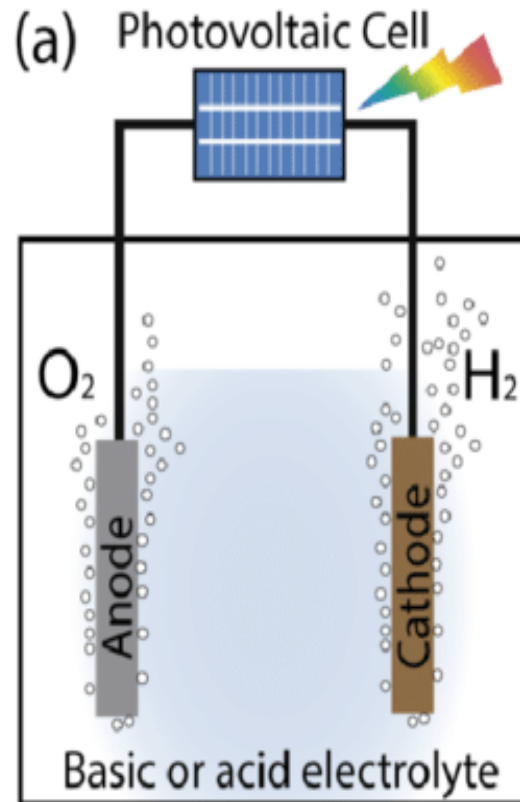
$$\eta_{\text{loss}} = \eta_{\text{resistance}} + \eta_{\text{OER}} + \eta_{\text{HER}}$$

**d**

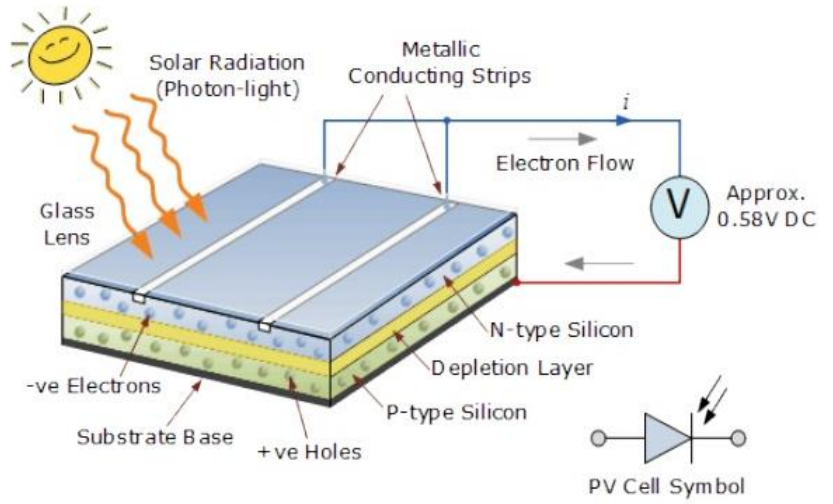
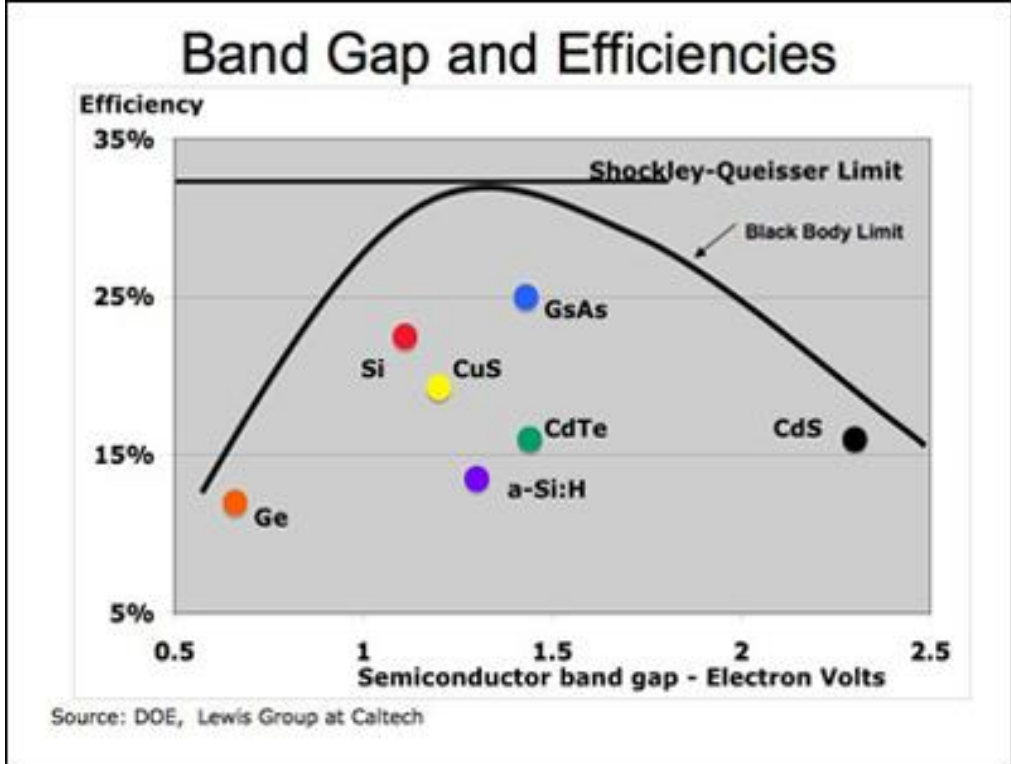
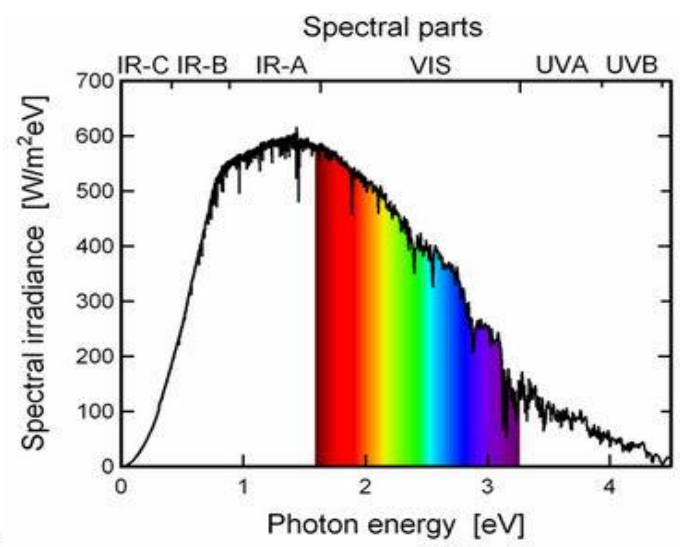
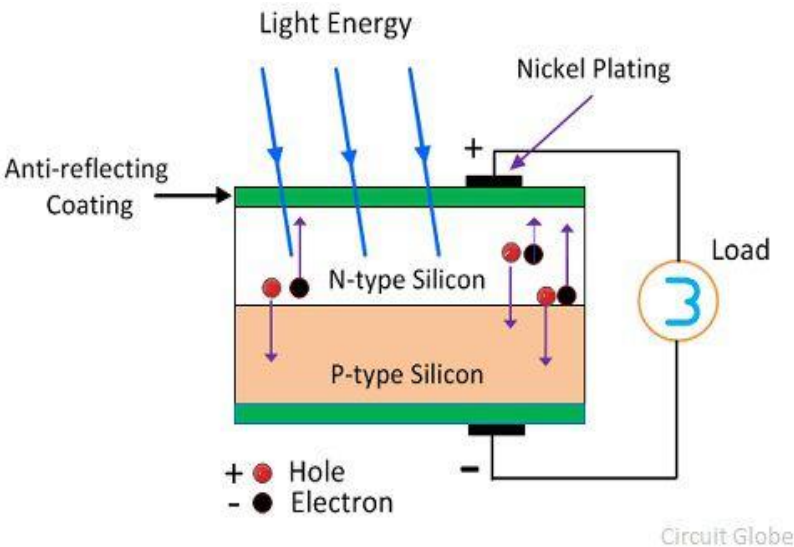


Célula fotovoltaica Si Externa

Célula Fotoeletroquímica (junto ao fotoanodo) formada por sistema gerador de elétrons ( $e^-$ ) e lacunas ( $h^+$ ) a partir da absorção de fótons



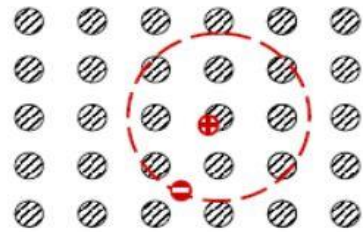
# LIMITES DE EFICIÊNCIA DA GERAÇÃO LIMITE DE SHOCKLEY-QUEISSER



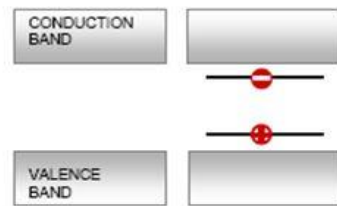
**PONTO CHAVE: SEPARAÇÃO DO EXCITON COM BAIXA RECOMBINAÇÃO DOS PORTADORES DE CARGA**  
**EXCITON → e<sup>-</sup> + h<sup>+</sup>**

**TIPOS DE EXCITONS:**  
**WANNIER** (SEMICONDUCTORES)  
**FRENKEL** (MATERIAIS E COMPOSTOS ORGÂNICOS)

**Wannier exciton**  
 (typical of inorganic  
 semiconductors)



SEMICONDUCTOR PICTURE



GROUND STATE    WANNIER EXCITON

**binding energy ~10meV**  
**radius ~100Å**

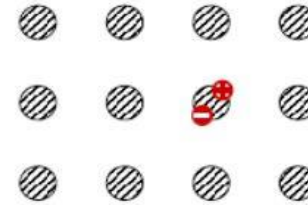
**Excitons**  
 (bound  
 electron-hole  
 pairs)

treat excitons  
 as **chargeless**  
**particles**  
 capable of  
 diffusion,

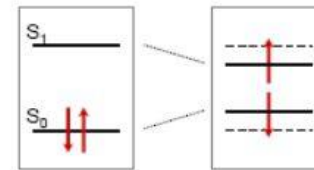
also view  
 them as  
 excited states  
 of the  
 molecule

**Charge Transfer (CT)  
 Exciton**  
 (typical of organic  
 materials)

**Frenkel exciton**  
 (typical of organic  
 materials)



MOLECULAR PICTURE



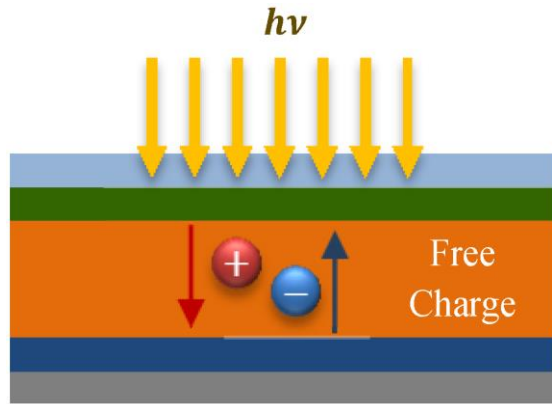
GROUND STATE    FRENKEL EXCITON

**binding energy ~1eV**  
**radius ~10Å**

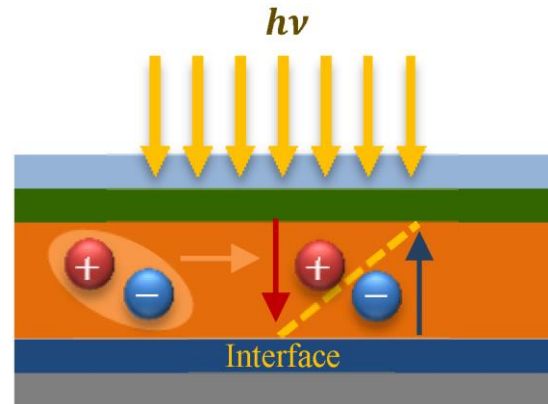
TIPOS DE CÉLULAS SOLARES E ESCALA TEMPORAL DOS PROCESSOS

Corantes orgânicos, polímeros conjugados, NP de semicondutores (CdTe)

Silício



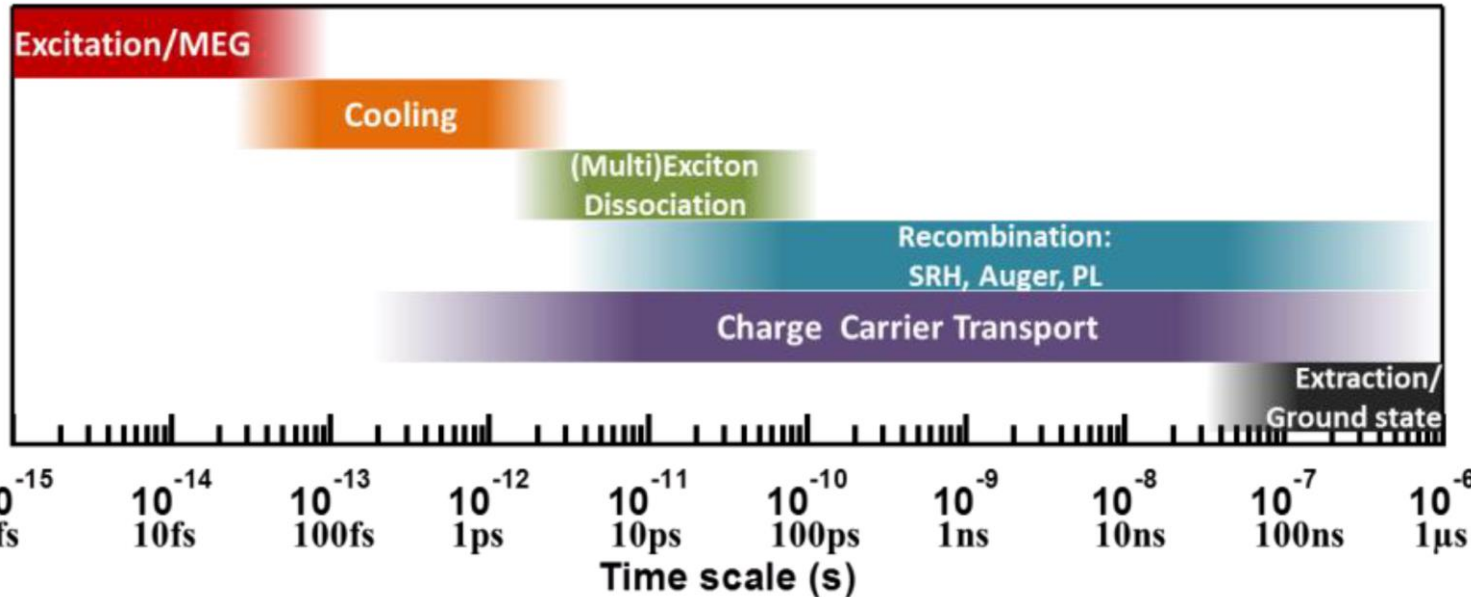
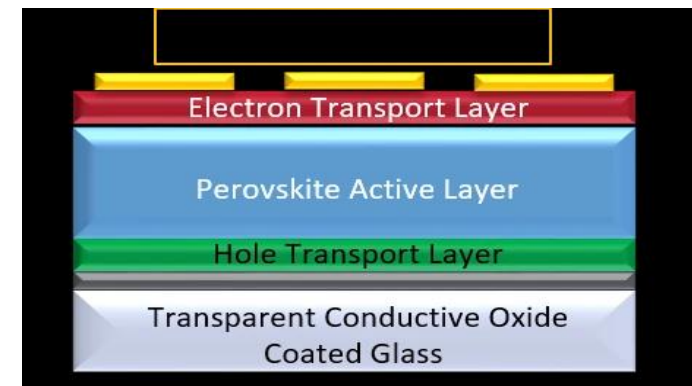
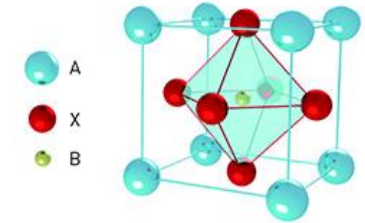
Conventional Solar Cell



Excitonic Solar Cell

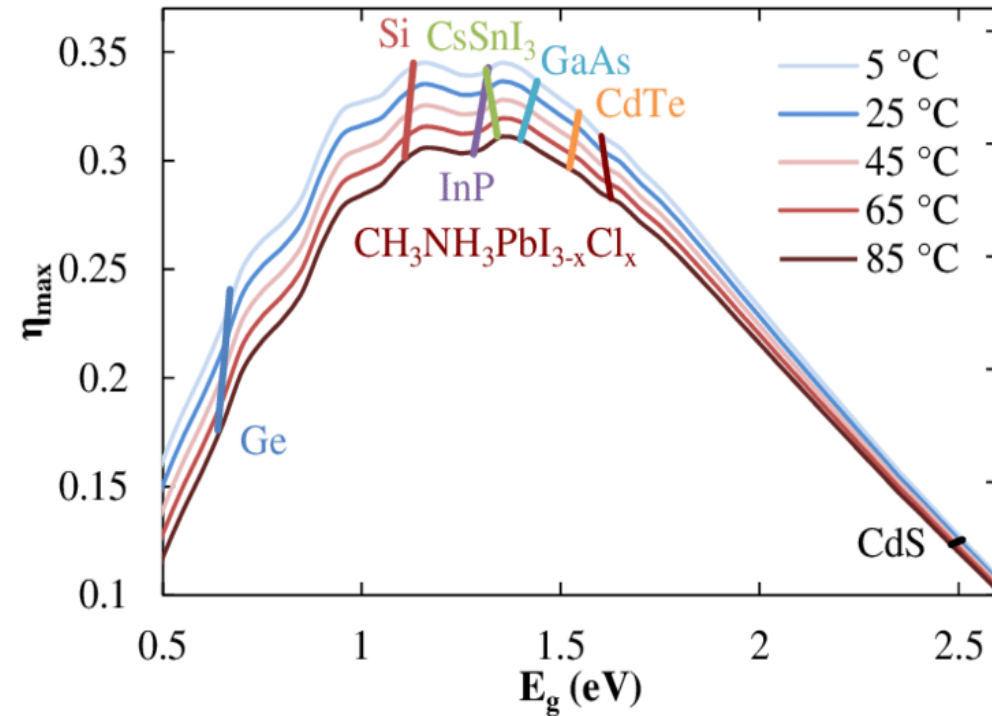
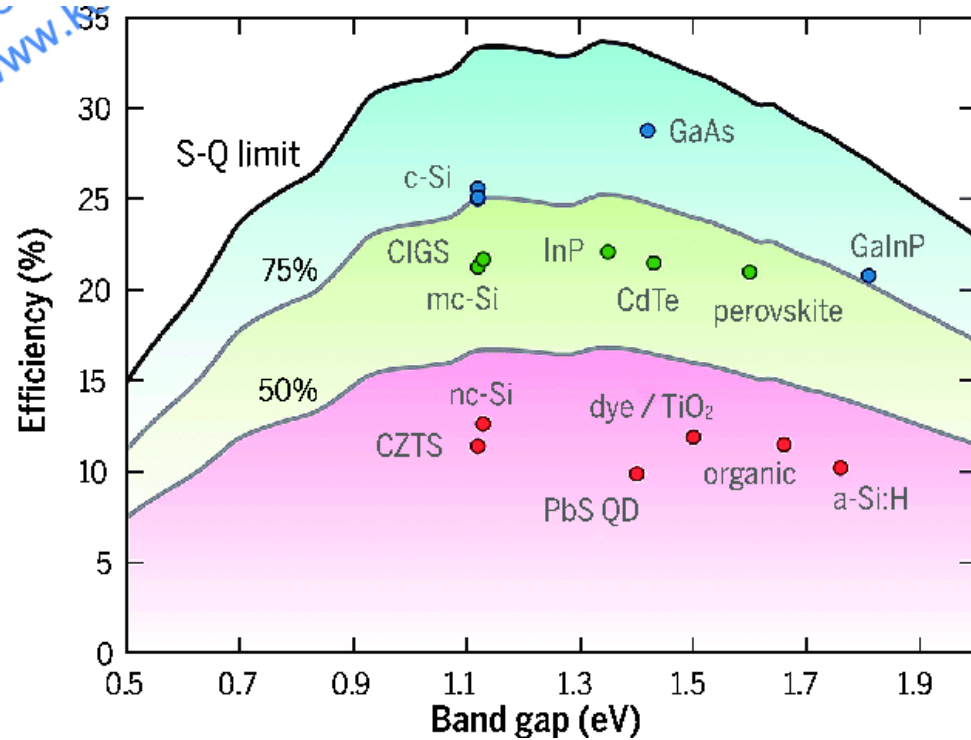
PEROVSKITAS

$ABX_3$ : B =  $Pb^{2+}$ , X =  $I^-$ , A = Cátion orgânico ( $NH_3^+$ ,  $CH_3NH_3^+$ )





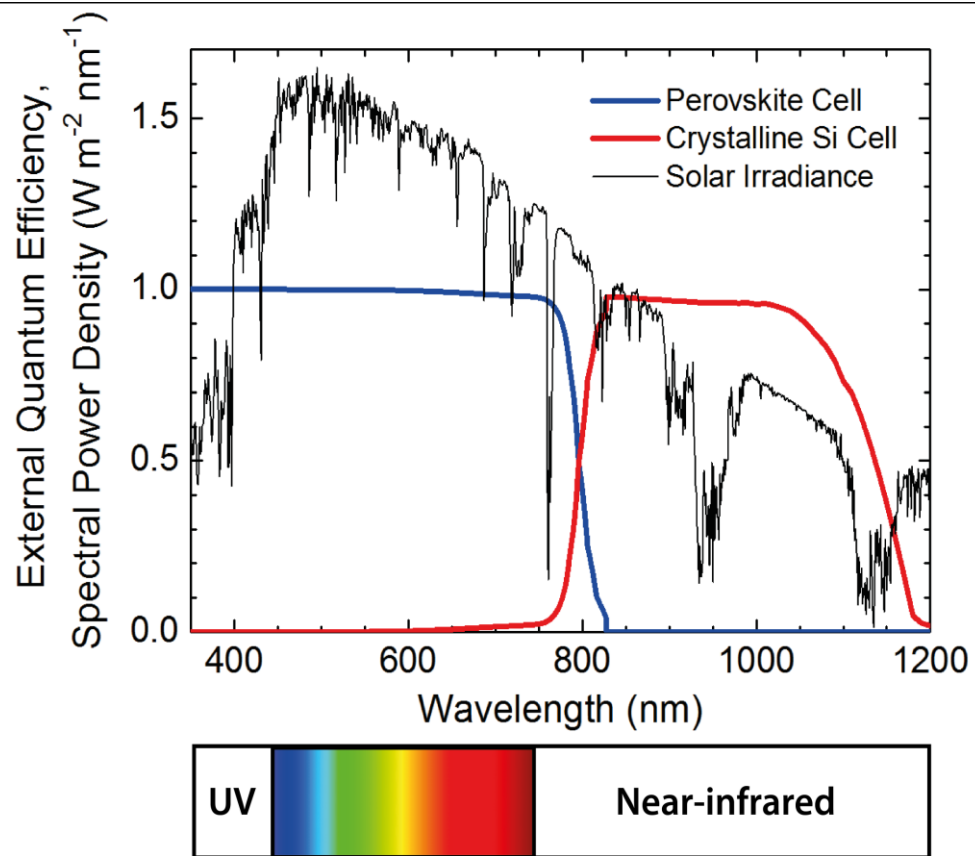
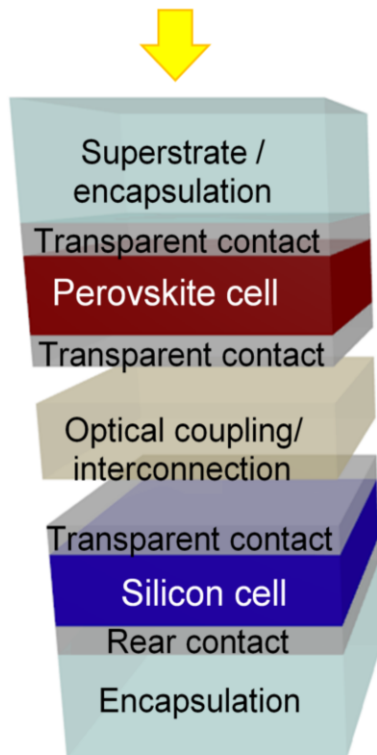
# EFICIÊNCIA COMPARATIVA



CONCLUSÃO: EFICIÊNCIA DE UMA ÚNICA CAMADA LIMITADA 1/3

QUESTÃO: COMO AUMENTAR A EFICIÊNCIA???

# COMBINAÇÃO DE SISTEMAS: CÉLULAS DE MÚLTIPLAS CAMADAS (TANDEM) PROMISSORA: PEROVSKITA + SILÍCIO

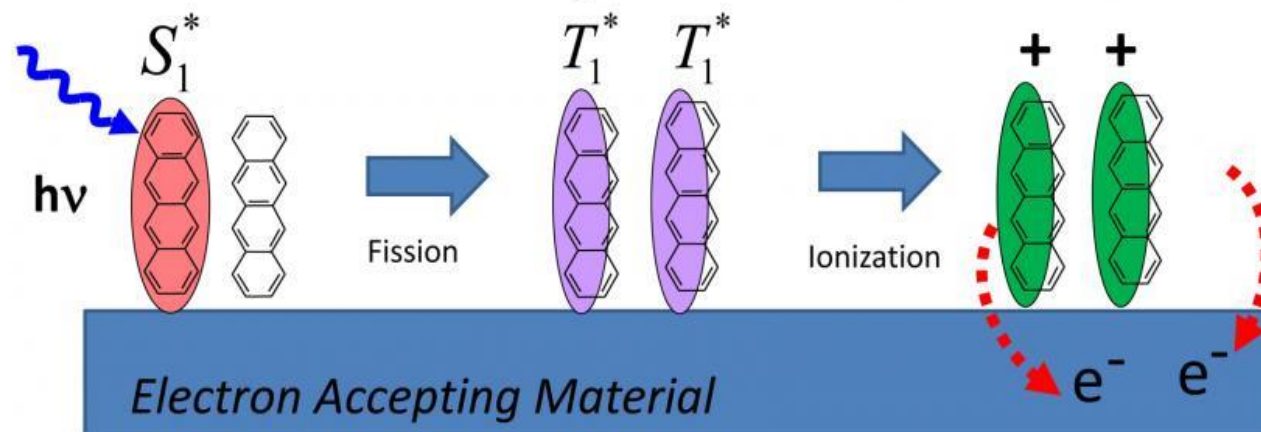


<https://www.epfl.ch/labs/pvlab/research/page-124775-en-html/>

COMO AUMENTAR AINDA MAIS O RENDIMENTO???

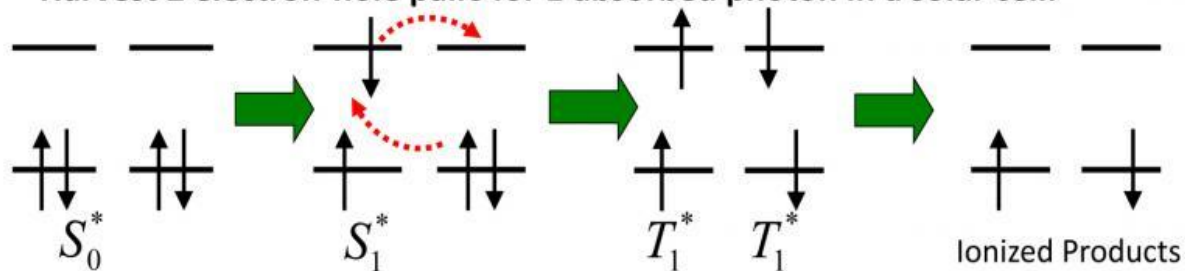
**RESPOSTA:** COMBINANDO PROCESSOS COM MAIOR EFICIÊNCIA DE GERAÇÃO DE PORTADORES DE CARGA (elétrons e lacunas)

Singlet Fission: 2 excitons for the price of 1 photon

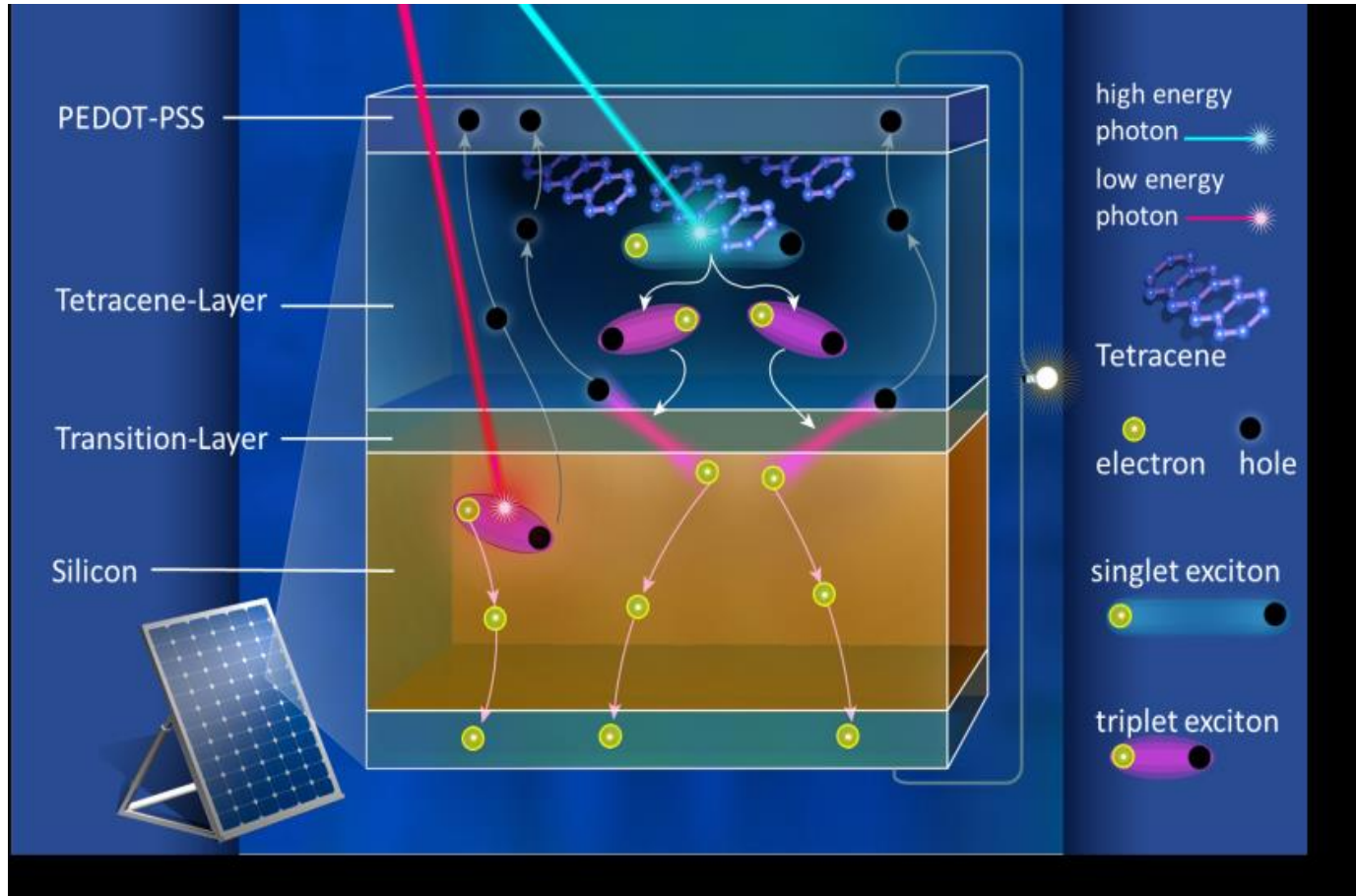


NANOCRISTAIS DE TETRACENO

Harvest 2 electron-hole pairs for 1 absorbed photon in a solar cell.

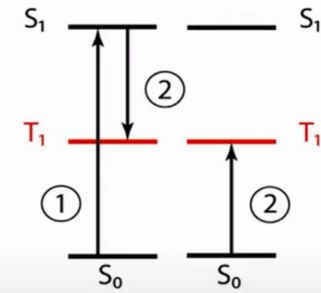


# MODELOS HÍBRIDOS (TANDEM CELLS)



Principle of a silicon singlet fission solar cell with incorporated organic crystals. (Source: M. Küsting / HZB)

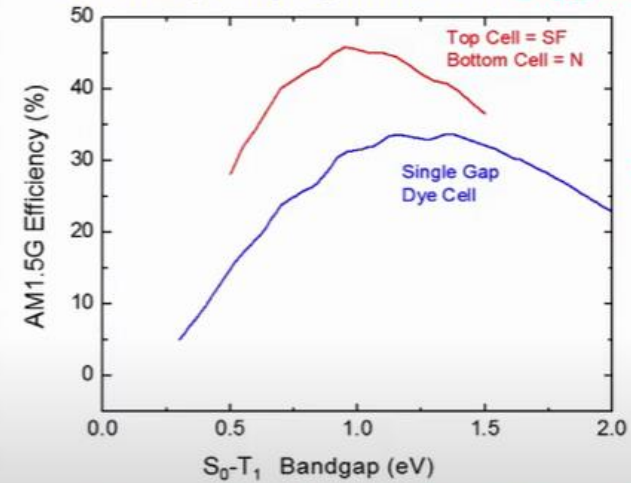
## SINGLET FISSION



spin allowed - **triplet yield up to 200%**  
**singlet fission is exoergic when  $\Delta E_S > 2 \Delta E_T$**   
**T-T annihilation is endoergic when  $\Delta E_Q, \Delta E_{T2}, \Delta E_S > 2 \Delta E_T$**

## SOLAR CELL: THEORETICAL EFFICIENCY

Ordinary single-junction vs. **singlet fission** solar cell



- Assumptions:**
- **200% triplet yield**
  - **each triplet yields e + h**
  - detailed balance
  - 1 Sun illumination
  - full absorption of incident solar light above 1.1 eV

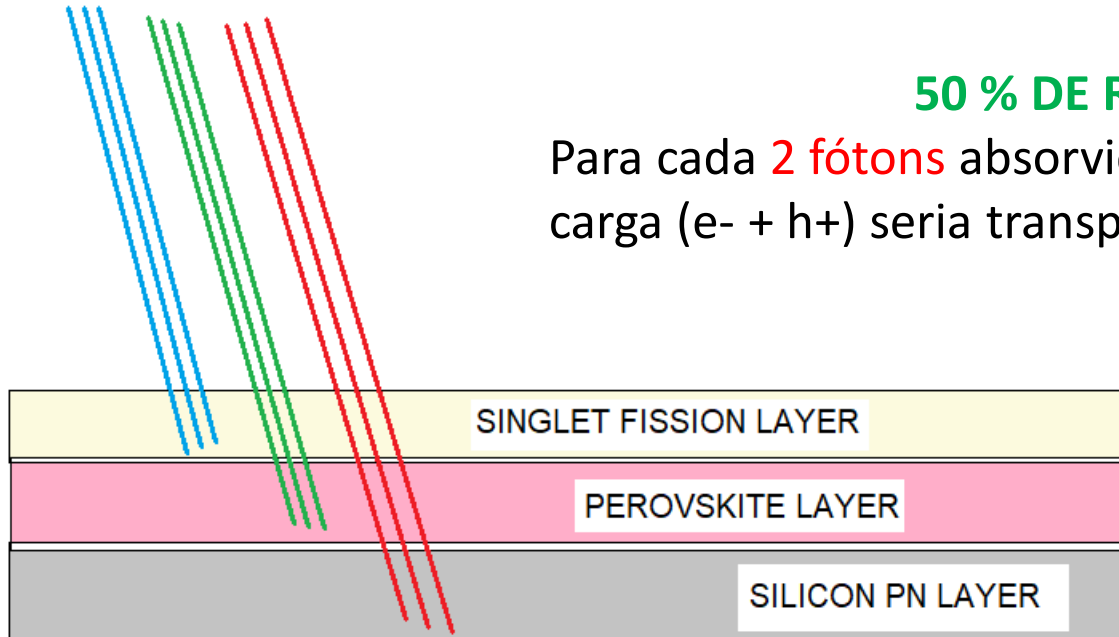
M. Hanna, A. J. Nozik, *J. Appl. Phys.* **2006**, *100*, 074510;

Shockley, W.; Queisser, H.J. *J. Appl. Phys.* **1961**, *32*, 510-519.

Fonte: Prof. J. Michl

QUAL SERÁ NO FUTURO A CÉLULA SOLAR DE ALTA EFICIÊNCIA ?

UV VISIBLE INFRARED



**50 % DE RENDIMENTO !!**

Para cada **2 fótons** absorvidos **uma** separação efetiva de carga ( $e^- + h^+$ ) seria transportado para corrente elétrica

QUÍMICA + FÍSICA + ENGENHARIA  
ENGENHARIA MOLECULAR