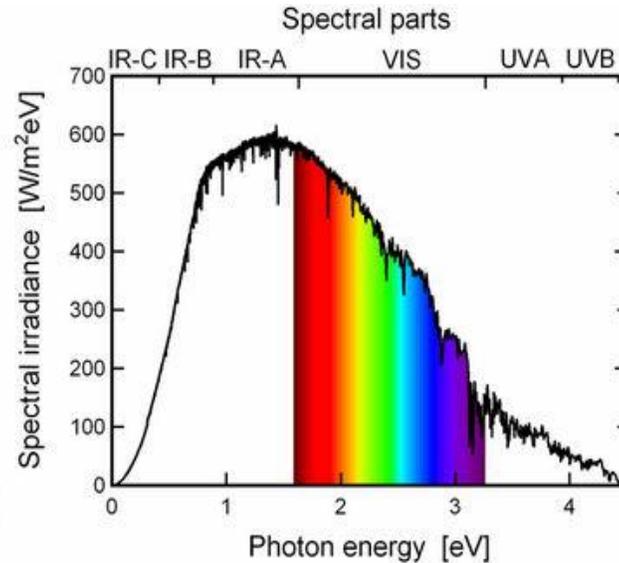
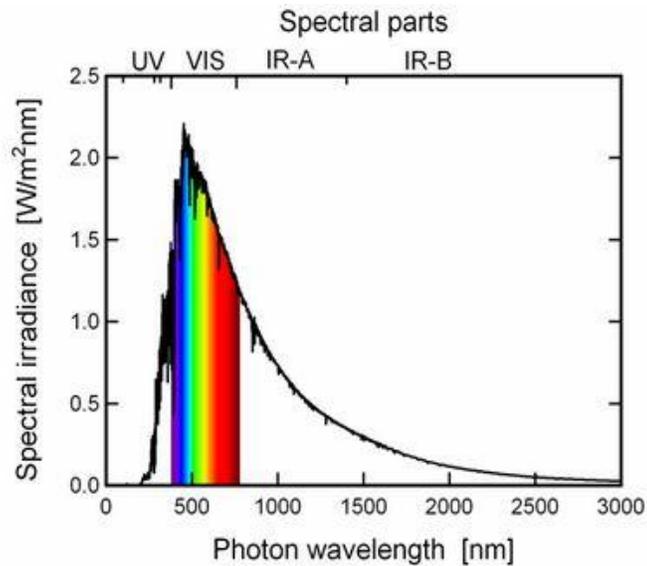
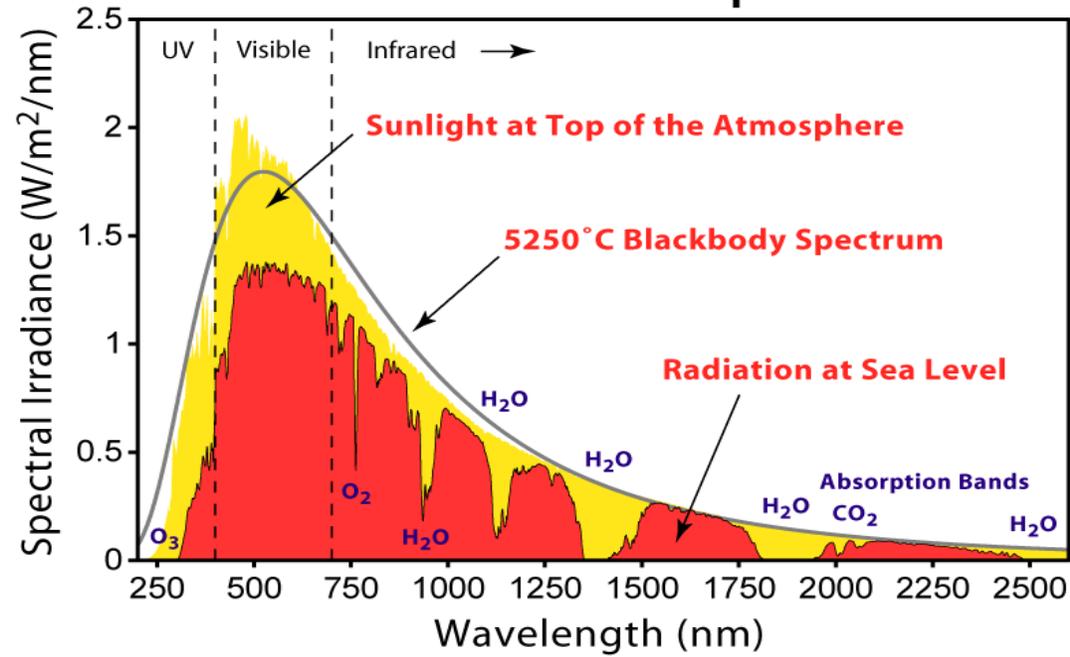


Solar Radiation Spectrum



COMO APROVEITAR A ENERGIA SOLAR???

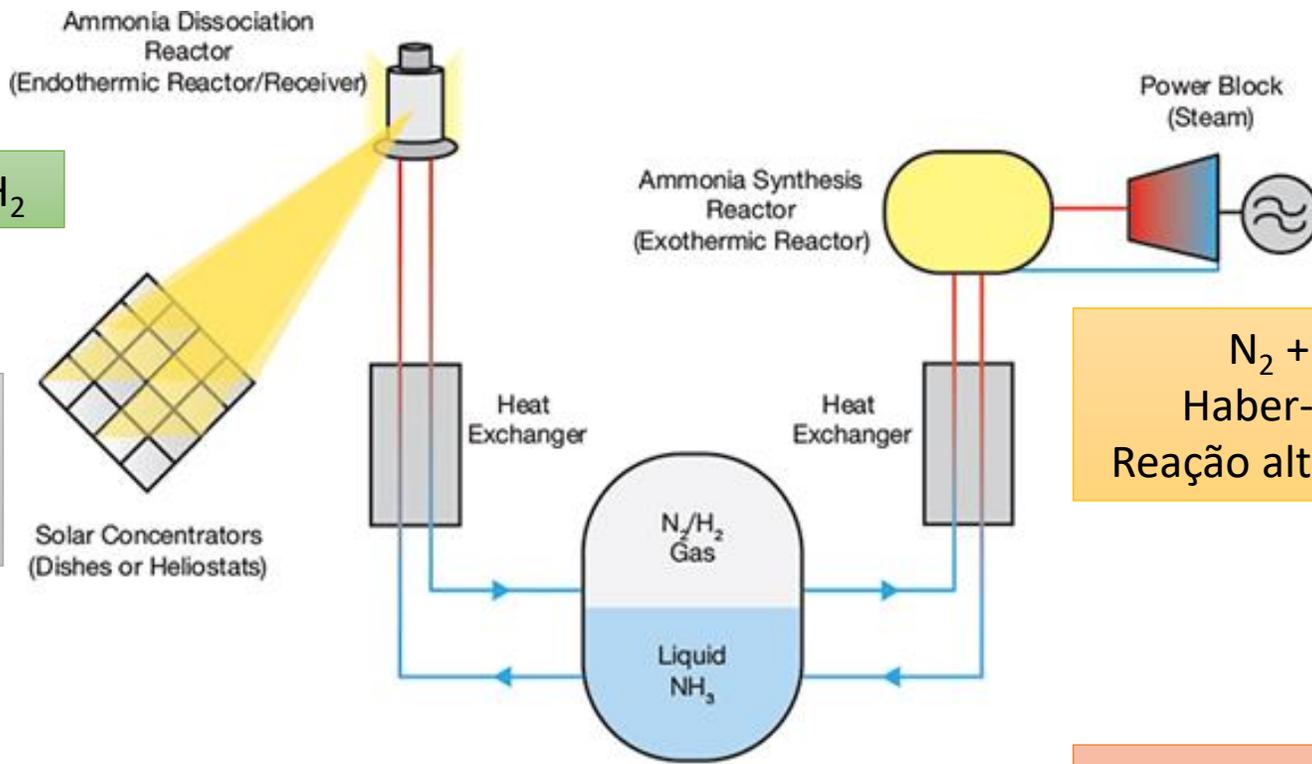
Uso de células fotovoltaicas
a base de Si



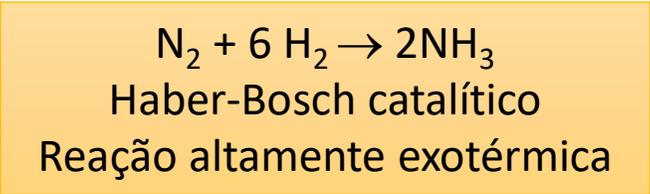
OUTRAS FORMAS DE UTILIZAÇÃO DA ENERGIA SOLAR
CICLO DA AMÔNIA (NH₃)
Ciclo termoquímico catalítico



Espelho parabólico para concentrar a radiação solar



Gerador de trabalho mecânico convertido em elétrico

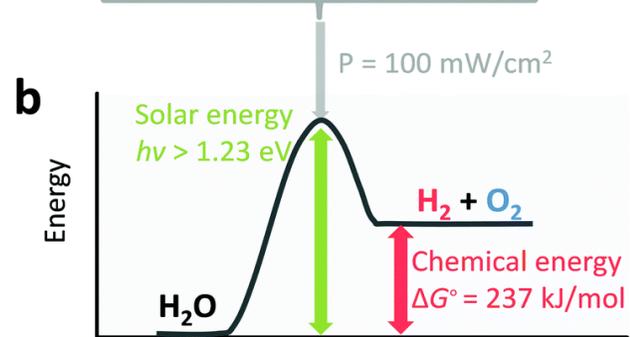
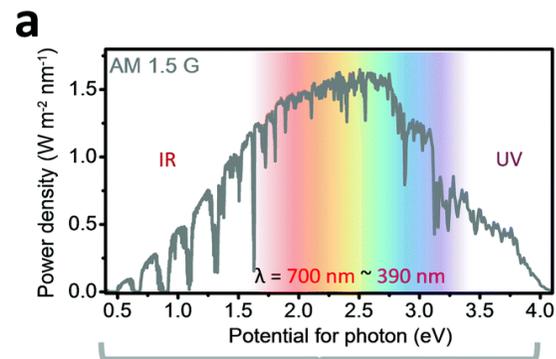


- Storage of Reactants at Ambient Temperature
- High-Pressure Underground Storage of Gases

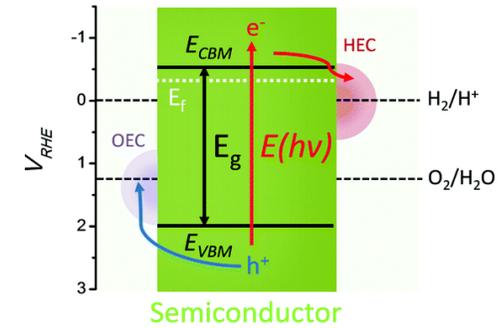
Problemas:
Escape de amônia
Alta pressão e temperatura
Escape de hidrogênio
Geração de óxidos de nitrogênio poluentes

<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
 $h\nu \geq 1,23 \text{ eV}$**



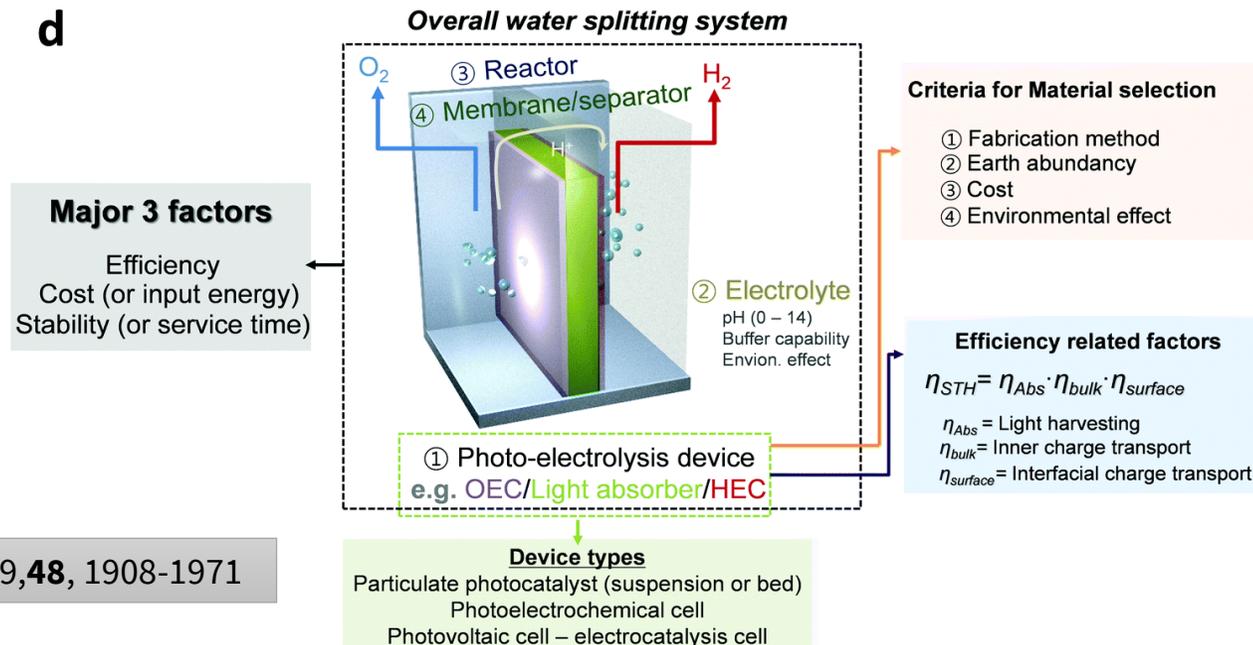
c Photon driven-water electrolysis



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

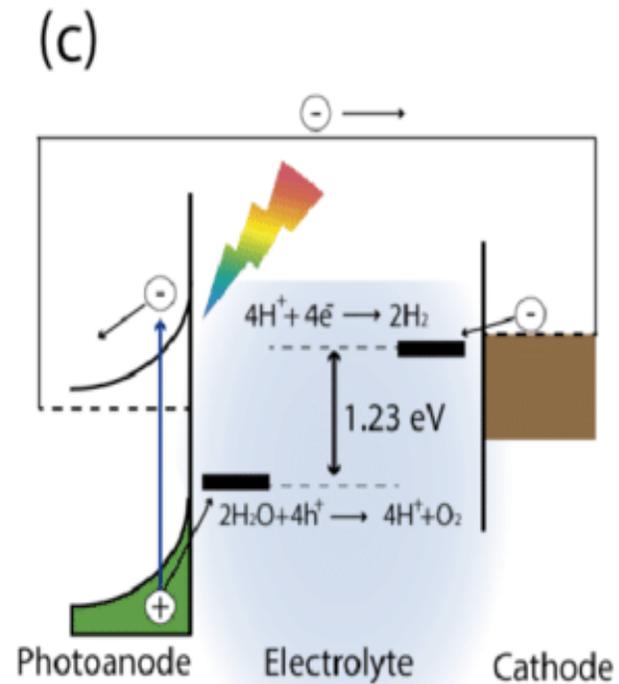
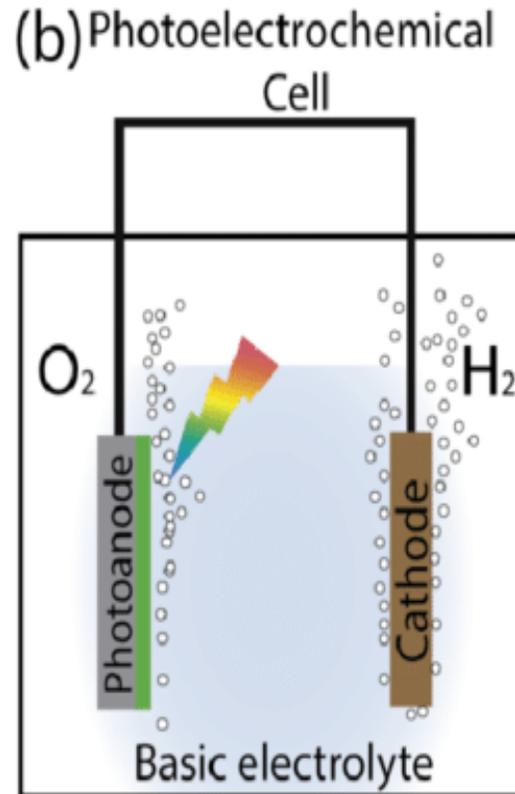
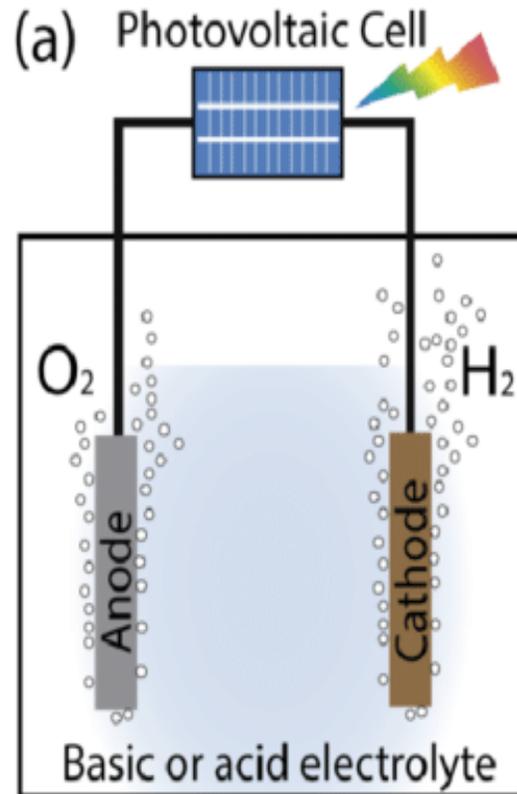
$$\eta_{\text{loss}} = \eta_{\text{resistance}} + \eta_{\text{OER}} + \eta_{\text{HER}}$$

d

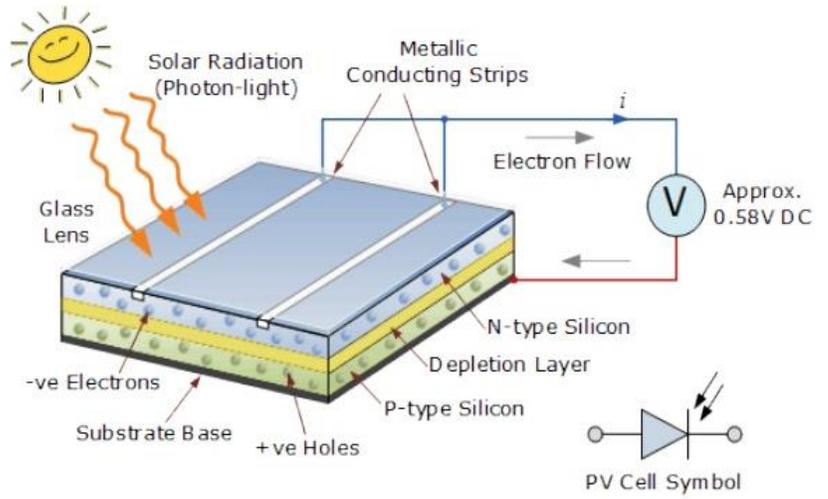
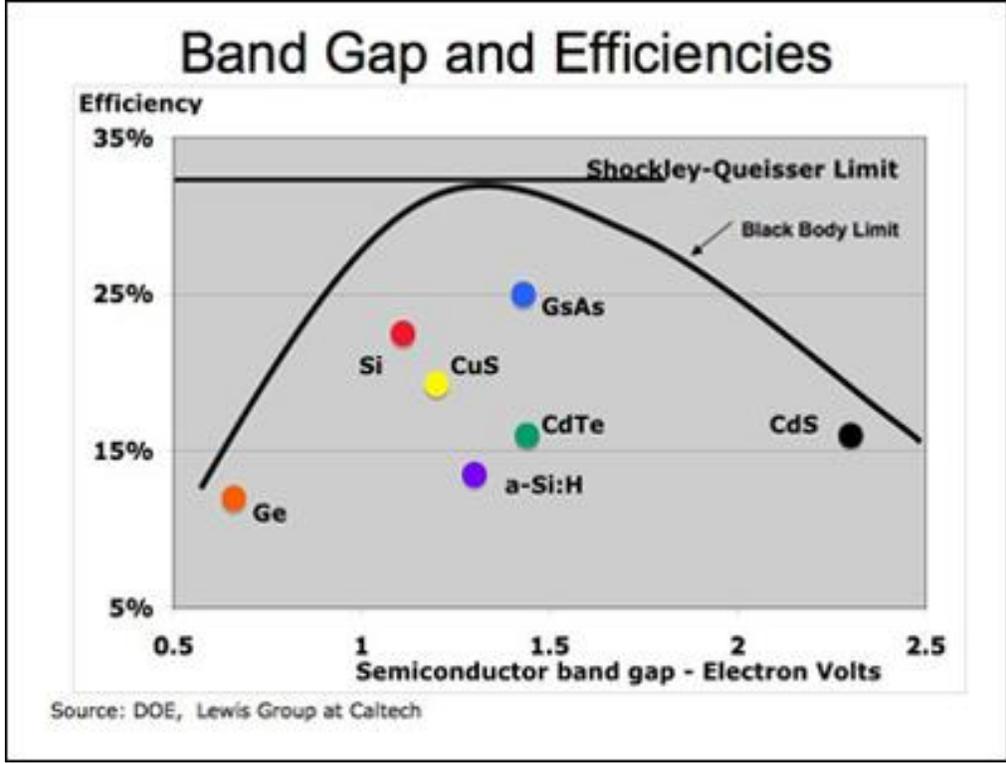
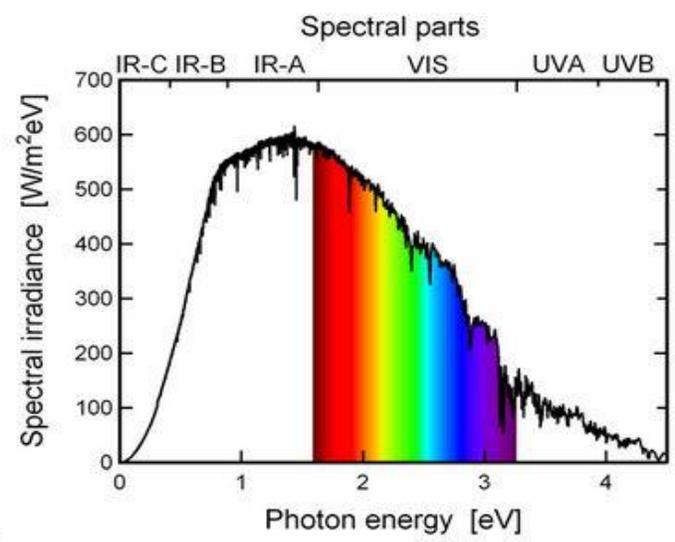
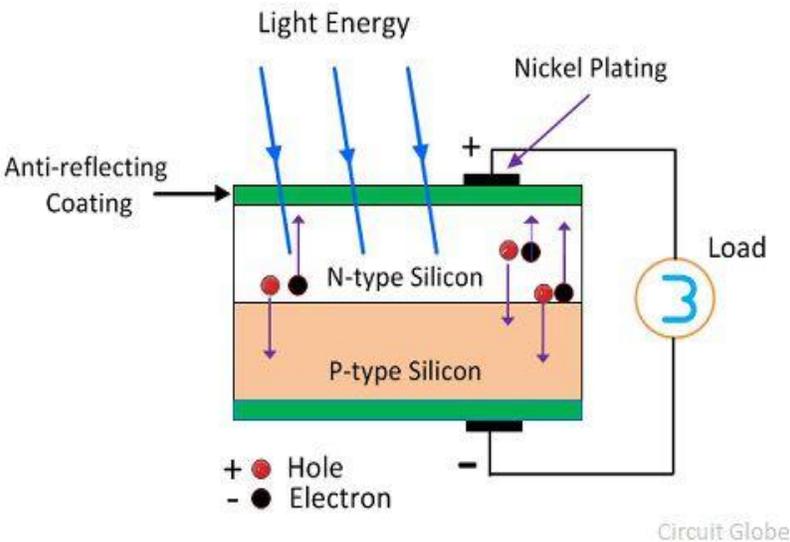


Célula fotovoltaica Si Externa

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



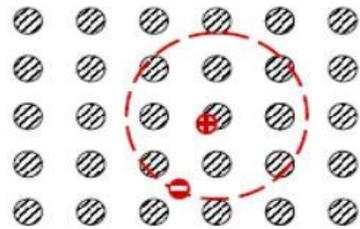
LIMITES DE EFICIÊNCIA DA GERAÇÃO LIMITE DE SHOCKLEY-QUEISSER



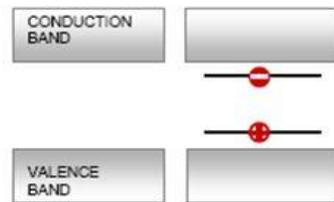
PONTO CHAVE: SEPARAÇÃO DO EXCITON COM BAIXA RECOMBINAÇÃO DOS PORTADORES DE CARGA
EXCITON → e⁻ + h⁺

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

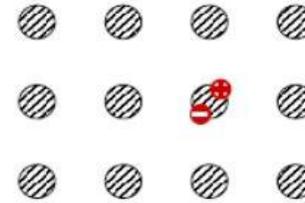
Excitons
 (bound
 electron-hole
 pairs)

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

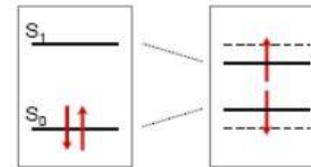
also view
 them as
 excited states
 of the
 molecule

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

Frenkel exciton
 (typical of organic
 materials)



MOLECULAR PICTURE



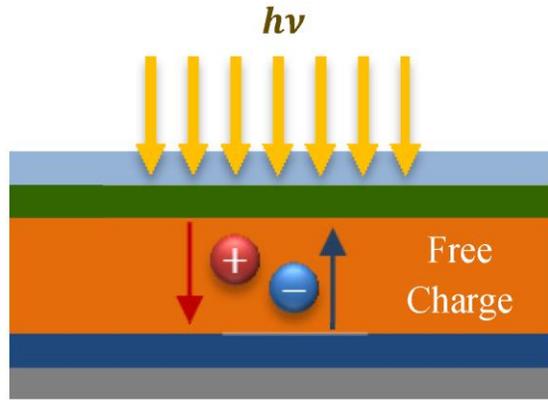
GROUND STATE FRENKEL EXCITON

binding energy ~1eV
radius ~10Å

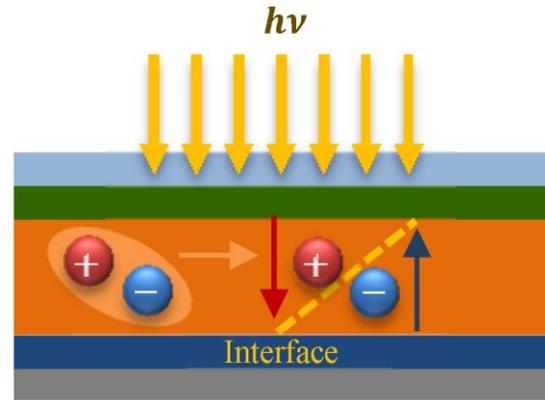
TIPOS DE CÉLULAS SOLARES E ESCALA TEMPORAL DOS PROCESSOS

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

Silício

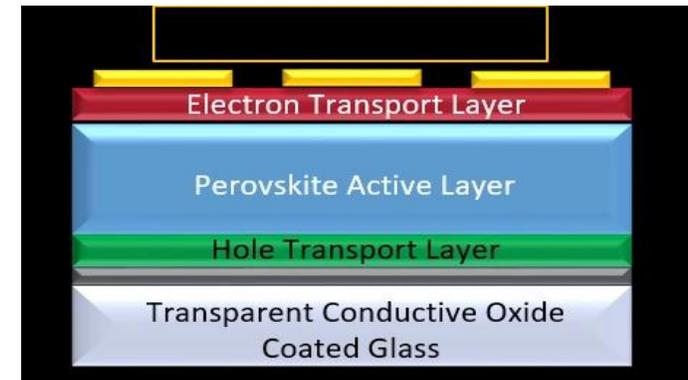
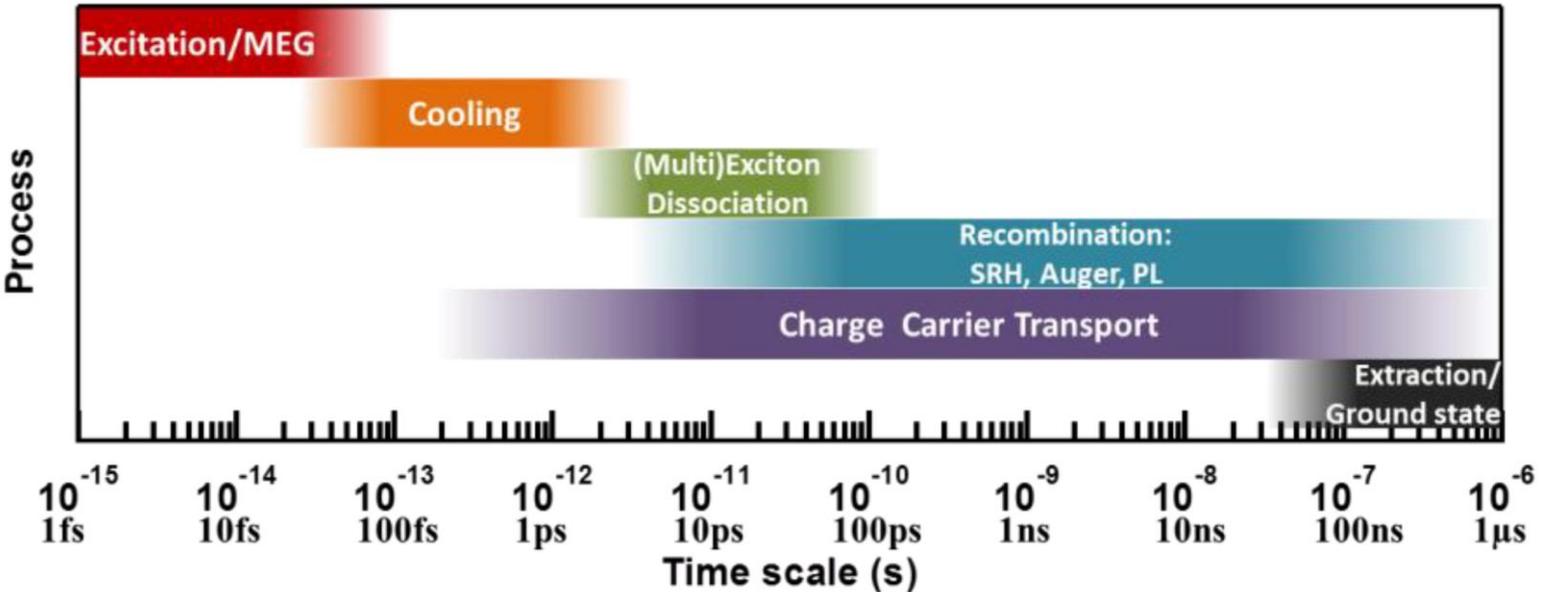
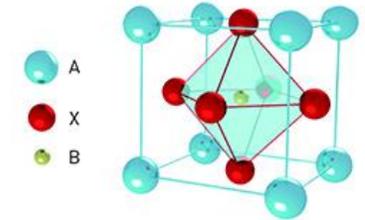


Conventional Solar Cell

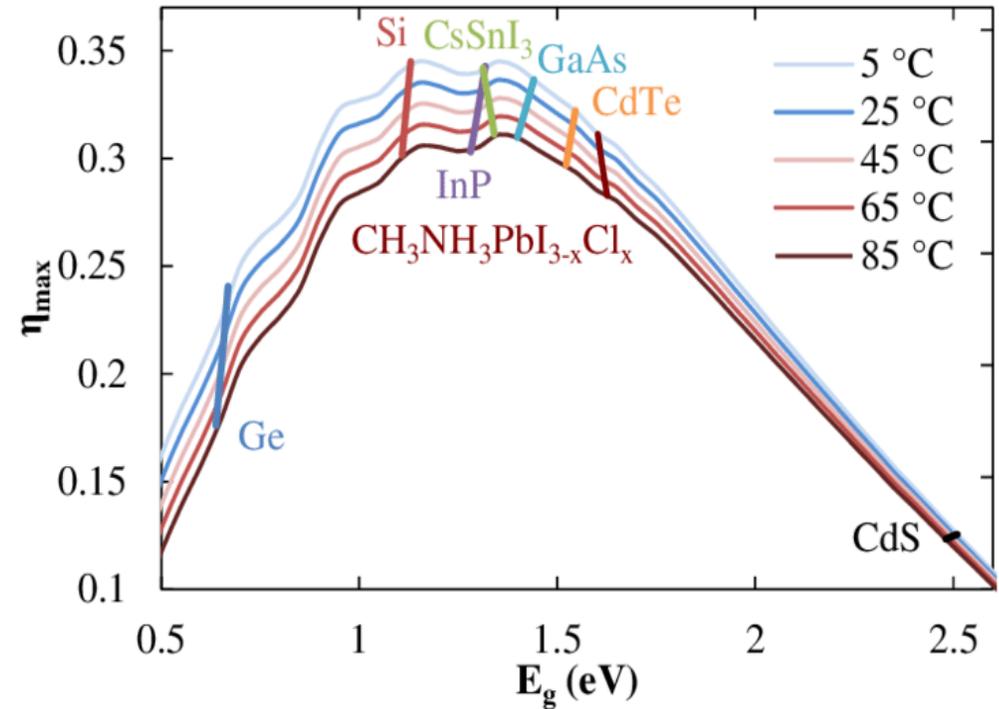
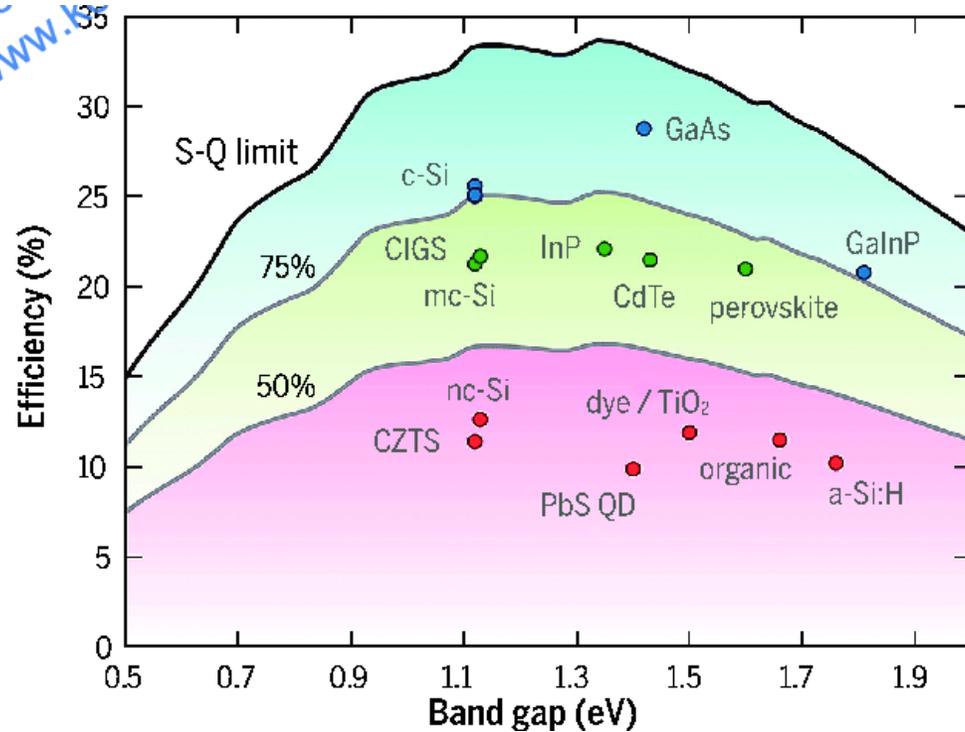


Excitonic Solar Cell

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



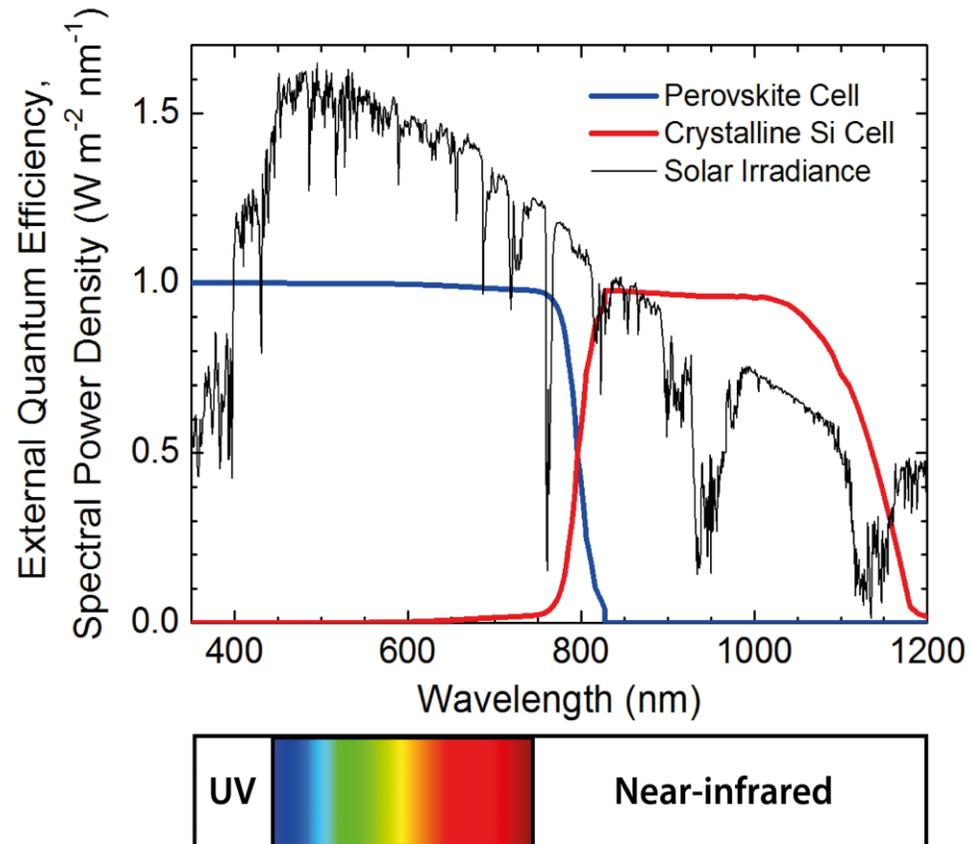
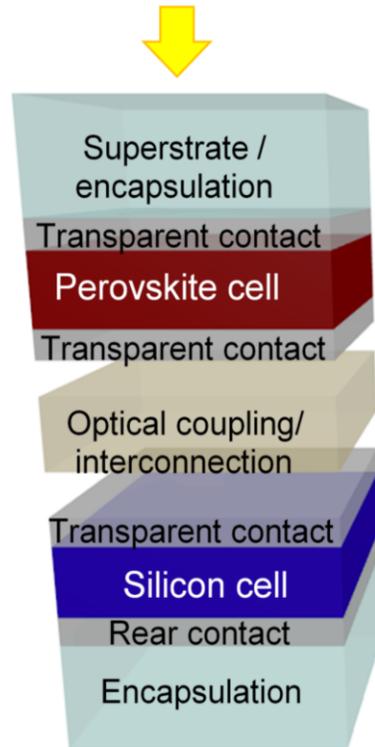
EFICIÊNCIA COMPARATIVA



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

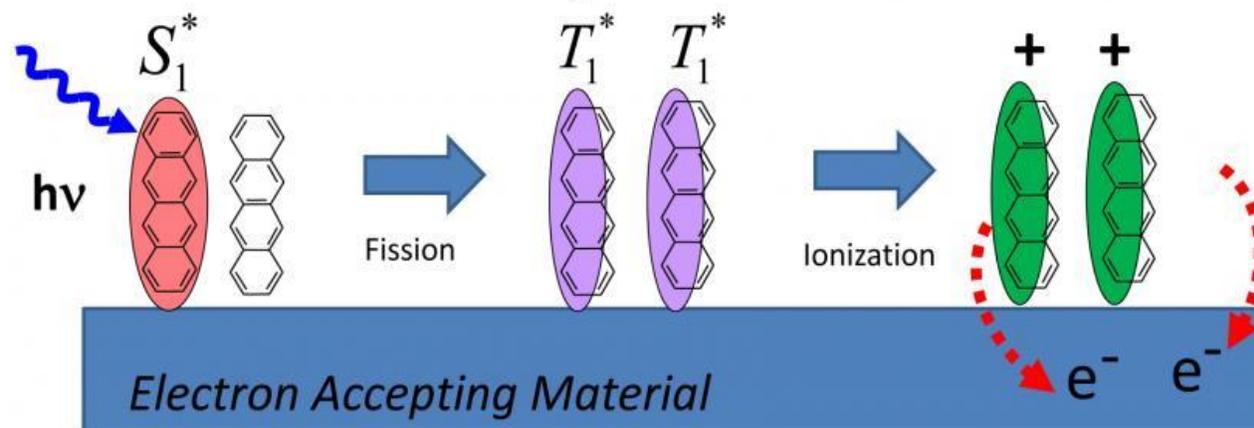


<https://www.epfl.ch/labs/pvlab/research/page-124775-en-html/>

COMO AUMENTAR AINDA MAIS O RENDIMENTO???

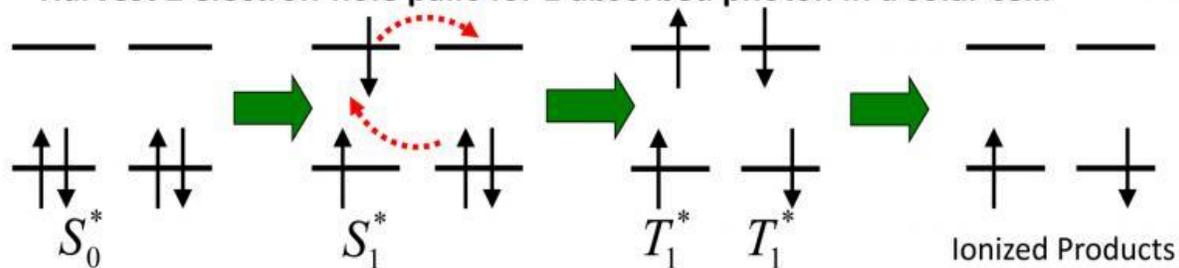
RESPOSTA: COMBINANDO PROCESSOS COM MAIOR EFICIÊNCIA DE GERAÇÃO DE PORTADORES DE CARGA (elétrons e lacunas)

Singlet Fission: 2 excitons for the price of 1 photon

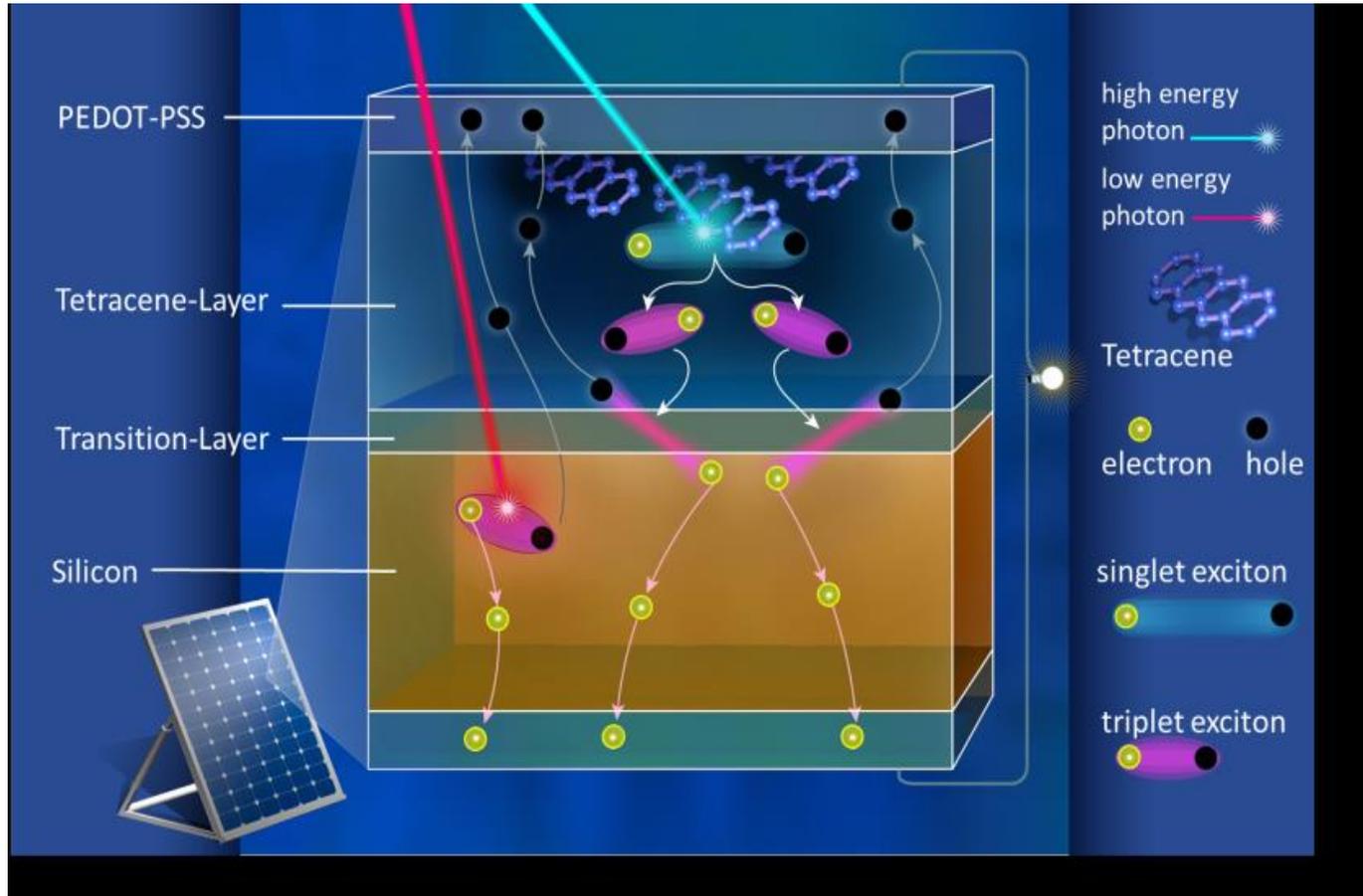


NANOCRISTAIS DE TETRACENO

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

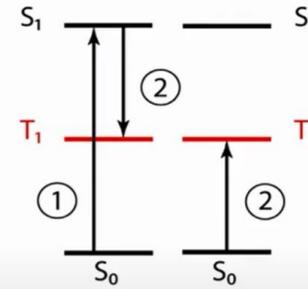


MODELOS HÍBRIDOS (TANDEM CELLS)



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

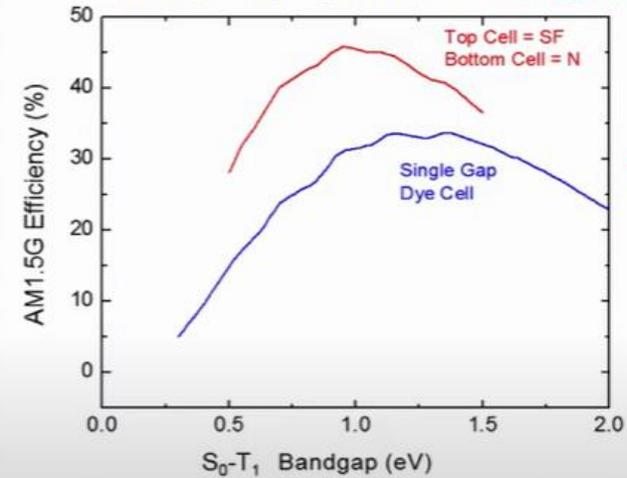
SINGLET FISSION



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

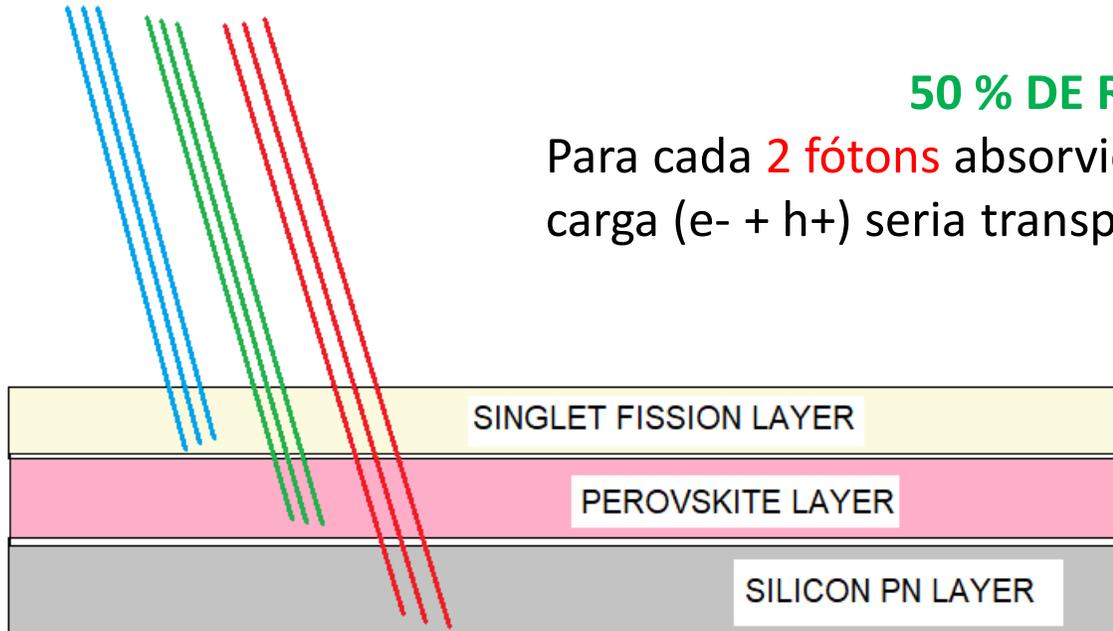
M. Hanna, A. J. Nozik, *J. Appl. Phys.* **2006**, *100*, 074510;

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