

Overview

Quokka3 tutorial slides



What is a Quokka?

A herbivorous marsupial,
native to South-Western
Australia.

Nocturnal and friendly,
with no fear of humans.

*"The happiest animal on
earth."*



Quokka: (silicon) solar cell simulator

- Quokka version 1 – 2¹
 - “Free and fast” 2D / 3D carrier transport in silicon solar cells
 - Developed at ANU, released 2013 on PV Lighthouse
 - Widely used in Si-PV community
- Quokka3²
 - Commercial successor released mid 2017
 - Developed during 2-year fellowship at Fraunhofer ISE



- Scientific partners:

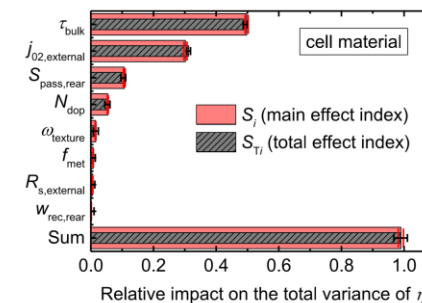
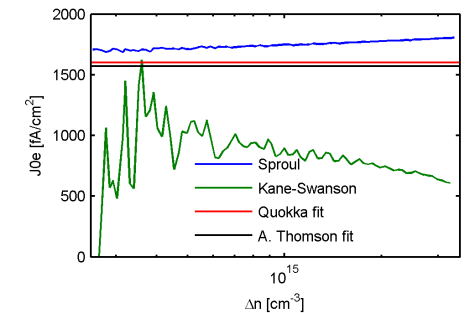
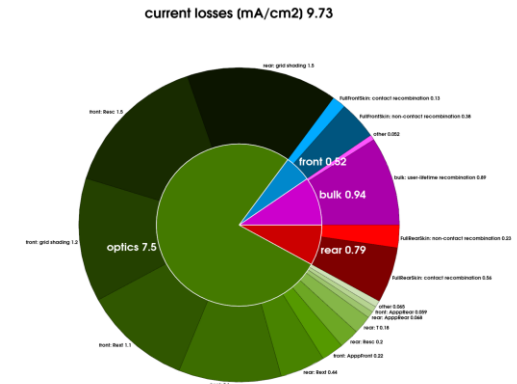
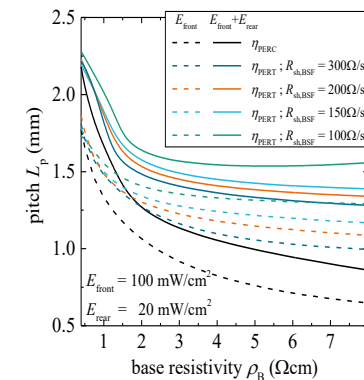


How modelling can help solar cell R&D

“Physical digital twin” of solar cell

- **Loss analysis** (quantify bottlenecks, road-mapping)
- **Find design optima** (e.g. optimum finger number)
- **Support characterization** (e.g. get J_{0e} from lifetime measurement)
- **Sensitivity analysis** (e.g. identify device property responsible for broad efficiency distribution)

Education on how a solar cell works

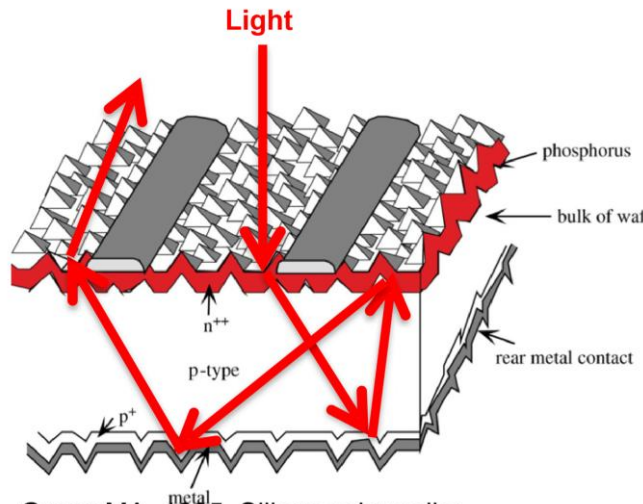


How to model a silicon solar cell

Solar cell = electro-optical semiconductor device

1. Optical modelling

Light reflection, scattering, absorption



Green MA, 1995, Silicon solar cells:
advanced principles and practice

2. Electrical modelling

Drift-diffusion carrier transport
Well established by IC industry

$$\frac{dn}{dt} = G - R_{el} - \nabla \vec{J}_{el} / q$$

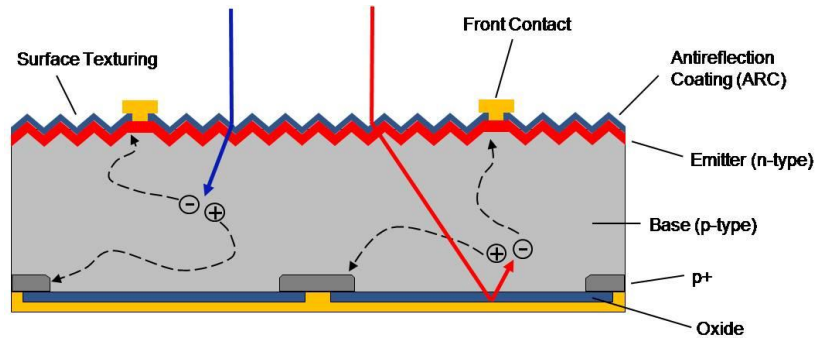
$$\frac{dp}{dt} = G - R_{hol} + \nabla \vec{J}_{hol} / q$$

$$\nabla(-\epsilon \nabla \phi_e) = \rho_{charge}$$

- Efficiency
- IV-curve
- sunsVoc-curve
- Reflection
- EQE / IQE
- PL / EL
- Loss breakdown
- ...



How to model a silicon solar cell



Detailed modelling

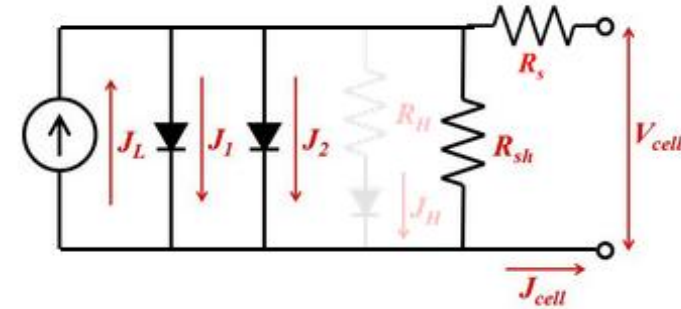
ray-tracing + full drift-diffusion



Highest insight and model accuracy



Expensive (cost, time, effort)



Lumped parameter modelling

two-diode model



Cheaper, quicker answers



Danger of over-simplification



"drift-diffusion" vs. "equivalent-circuit" bulk model type

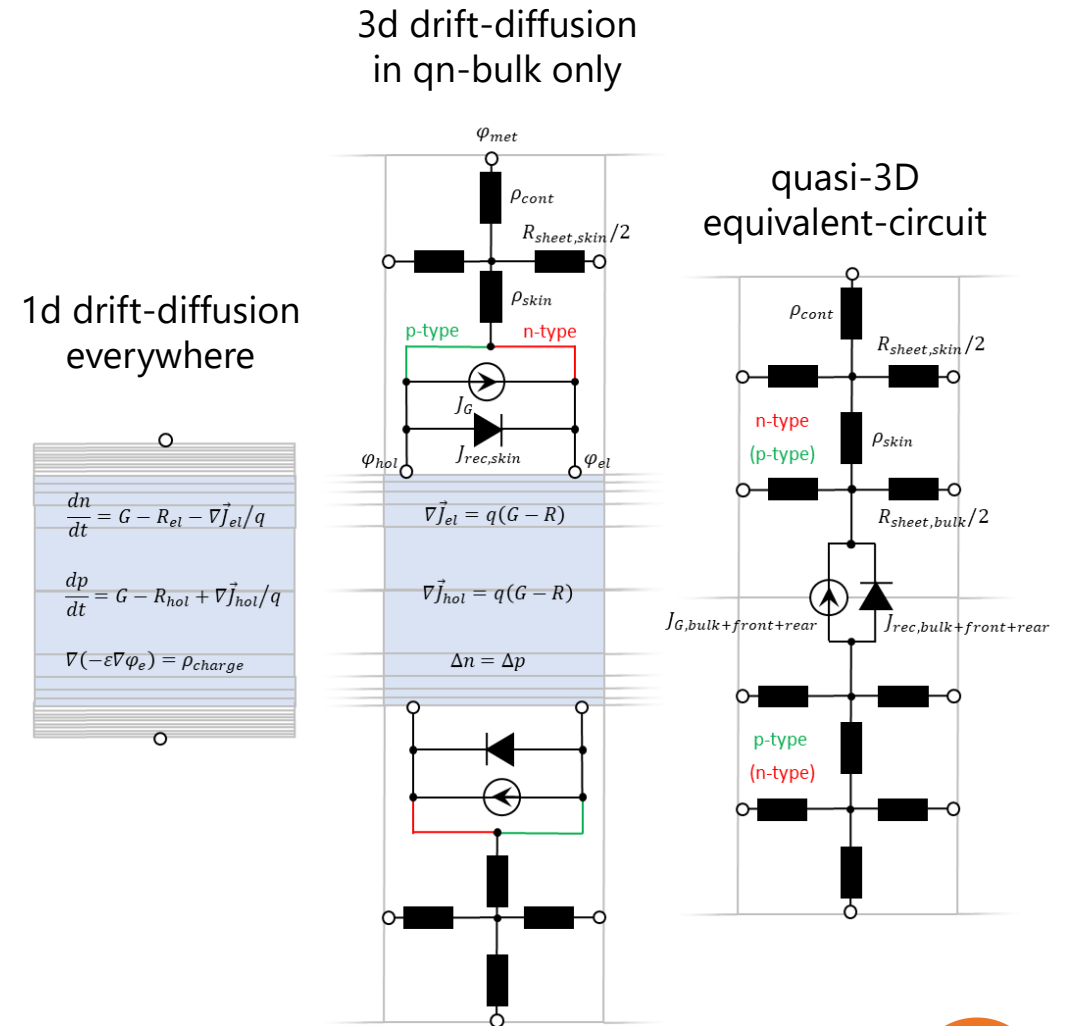
- Instead of drift-diffusion, bulk carrier transport can be simplified to an equivalent circuit model = "Distributed diode model"

- **Advantages of equivalent-circuit**

- No bulk mesh, much faster, much more robust
- Good for large geometric variations
- Simple setting option in Quokka3

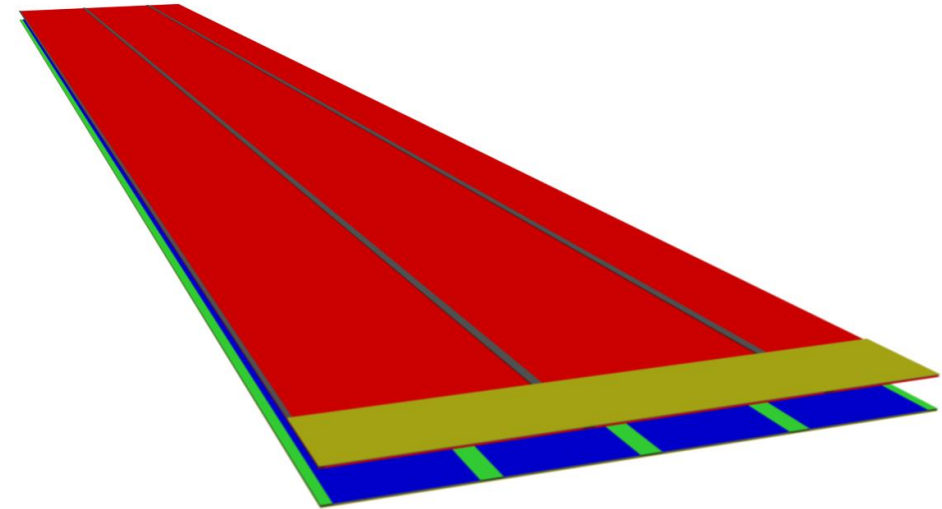
- **Disadvantages of equivalent-circuit**

- Assumes depth-uniform carrier profile
- No bulk collection loss, inaccurate current crowding at local contacts, ...
- Incompatible with IBC



concept of a solar cell in Quokka3

- **Bulk**
 - Main absorber, **quasi-neutral (qn) drift-diffusion**
- **Skins**
 - Thin regions including non-qn near-surface of bulk
- **Contact**
 - Defining where current can flow between skin and metal
- **Metal**
 - Ohmic current transport
- **Pads**



■ / ■ / ■ : n-type / p-type / non-conductive skin



What is a "skin"?^{1,2}

Thin region from a **quasi-neutral** position in the **bulk** close to the surface, **to** either the actual **surface** (non-contacted skin) or the interface to metal (contacted skin)

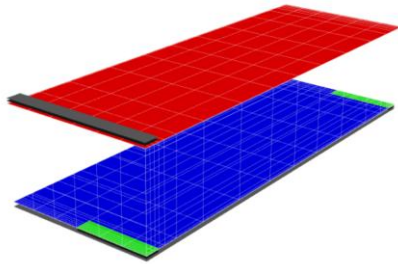
inversion layer

diffusion on textured surface

Si-perovskite tandem

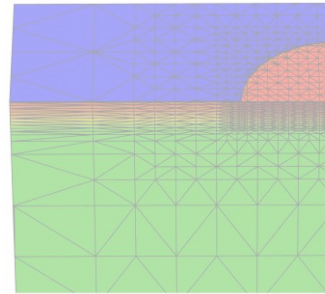


How to account for skins in solar cell modeling



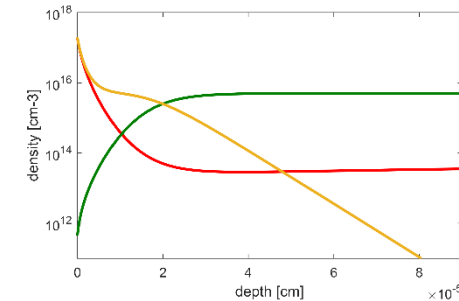
*Lumped **cell** modeling*

- $J_0 + R_{sheet}$ (+more)
- 2D / 3D: conductive boundary model¹
- Quokka / PC2D



*Full detailed **cell** modeling*

- Surface SRH + doping profile
- 1D: PC1D, Quokka3, ...
- 2D / 3D: commercial device simulation tools



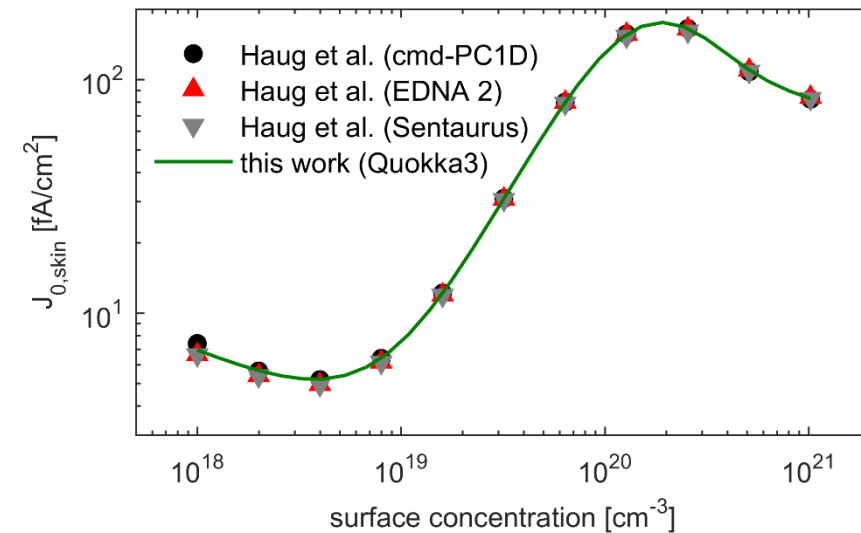
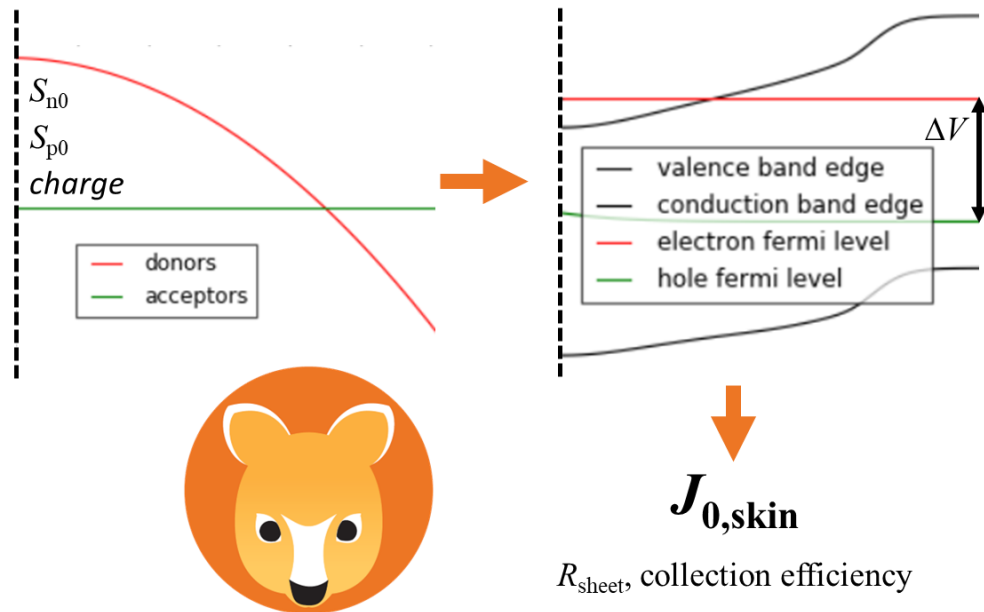
*Detailed **skin** modeling*

- (quasi)-1D
- Gives lumped parameters as result
- EDNA2 / Quokka3

Multiscale modeling²

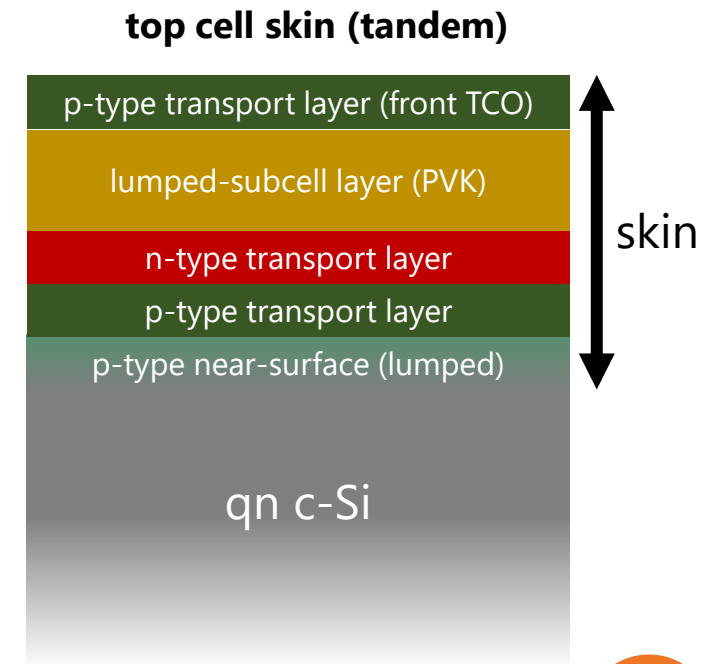
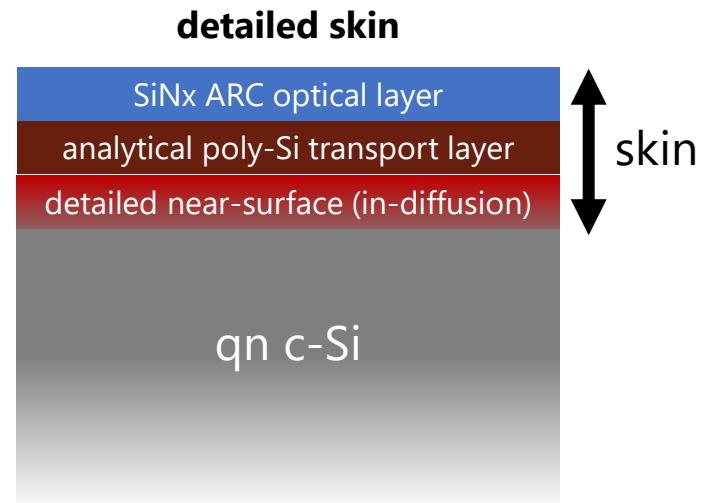
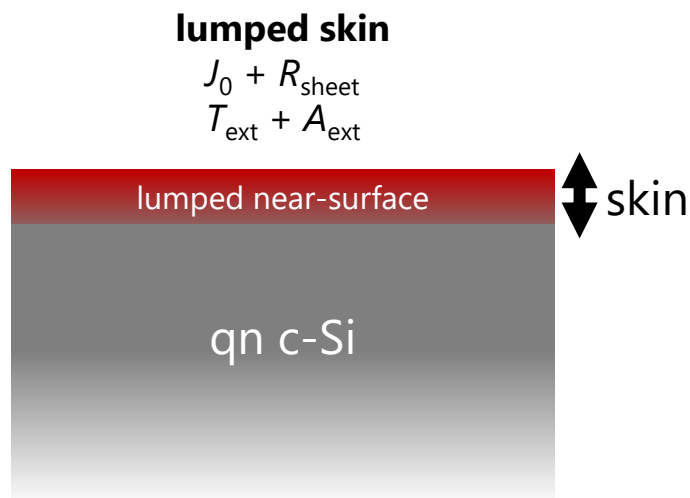


- Solving the full semiconductor equations in 1D (no qn assumption)
- Directly simulate $J_{0,skin}$ and collection efficiency of diffused junctions ($\sim$ EDNA)
- Extends to MIS-type contacts¹ and passivation with surface charge¹



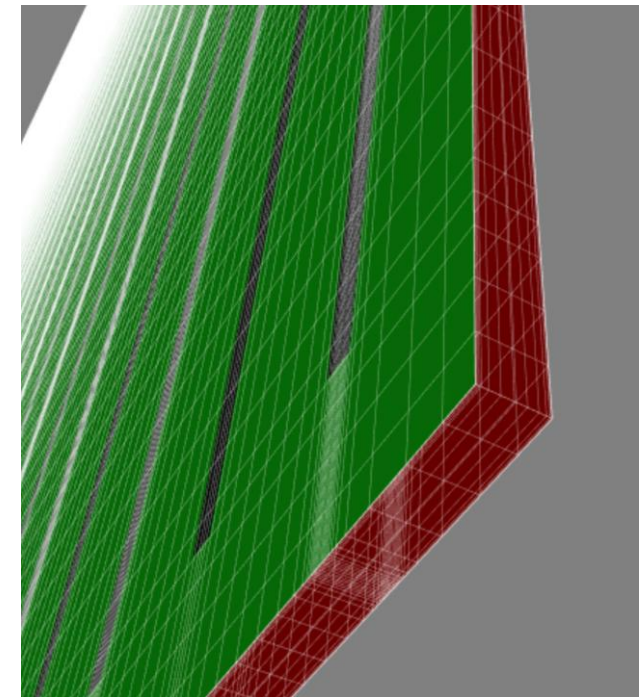
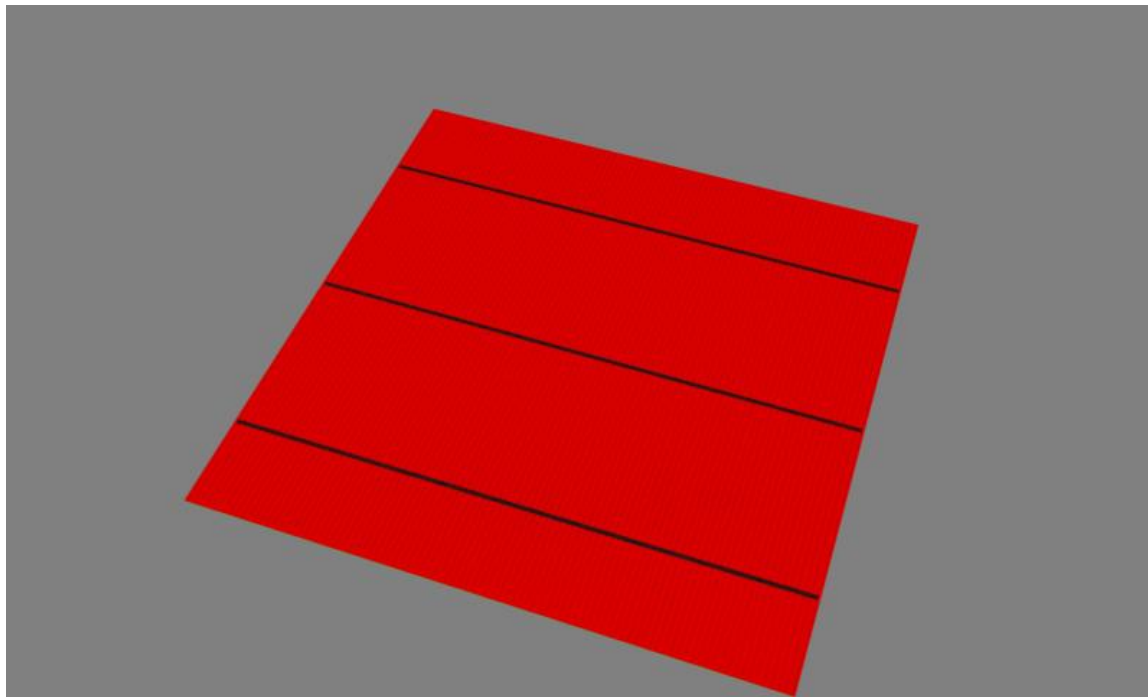
Skin layers in Quokka3

- A skin in Quokka3 can consist of multiple **layers**, supported types are:
 - **near-surface** layer (non-quasi-neutral part of Si wafer, modelled with drift-diffusion for detailed skin)
 - **transport** layer (electron OR hole conductive layer, analytically modelled)
 - **lumped-subcell** layer (top cell for tandem, characterized by JV and EQE curve)
 - **optical** layer (for detailed optical modelling via TMM)



Large 3D geometries

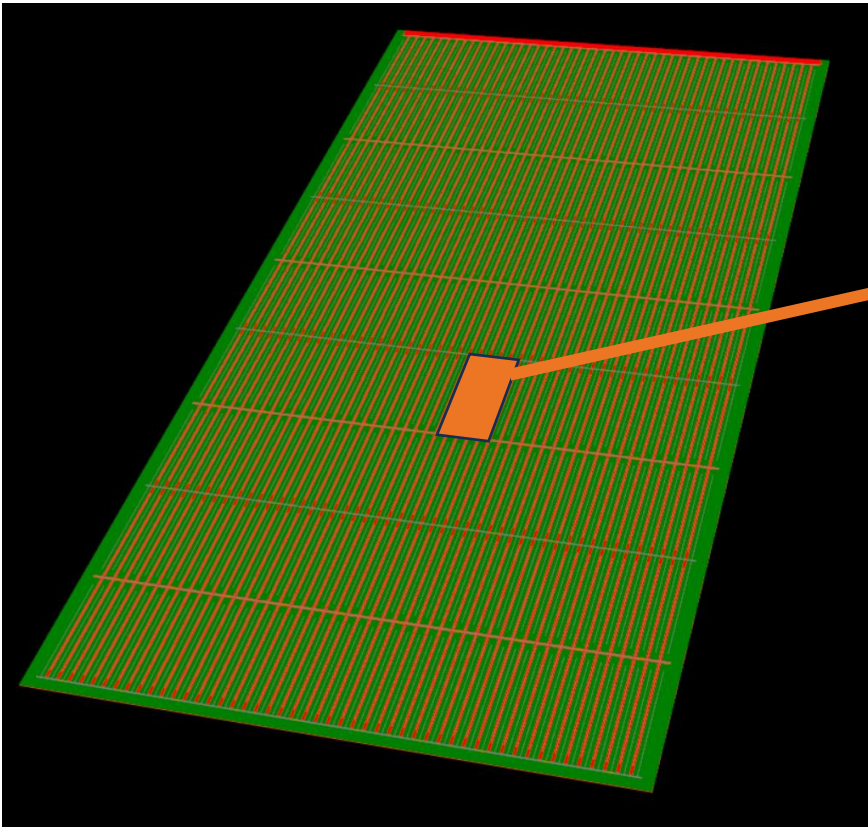
- Rebuild of "Quokka"-model in C++ -> **10x – 100x performance increase**
- Copes with up to millions of elements -> **up to a full 210mm cell in 3D**
- Includes current transport in **metal layer**



Full cell vs unit cell

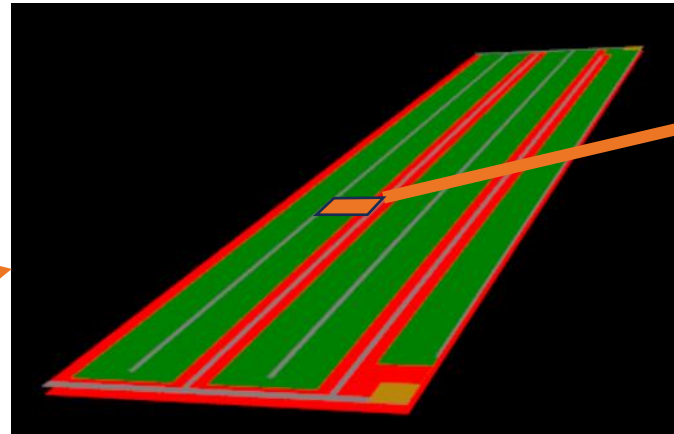
full-cell domain

Challenging to solve due to very large numerical mesh



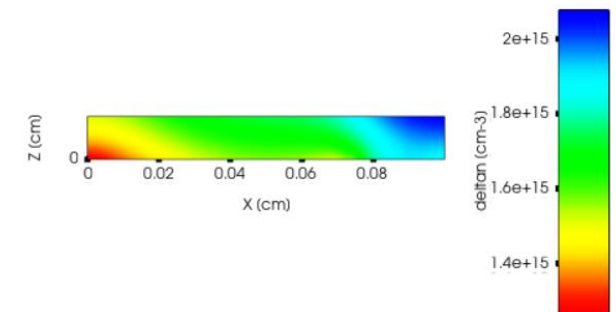
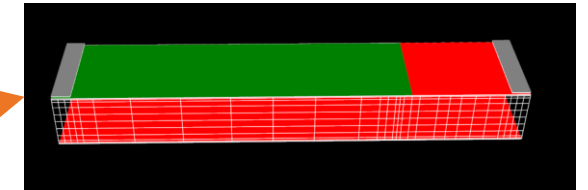
busbar-/pad-enhanced unit cell

neglects edge effects



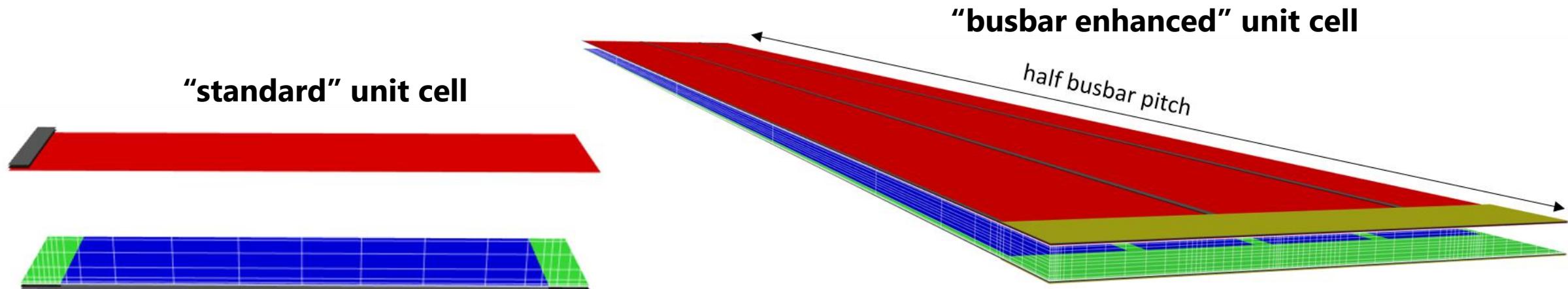
standard unit cell

neglects busbars, finger resistance



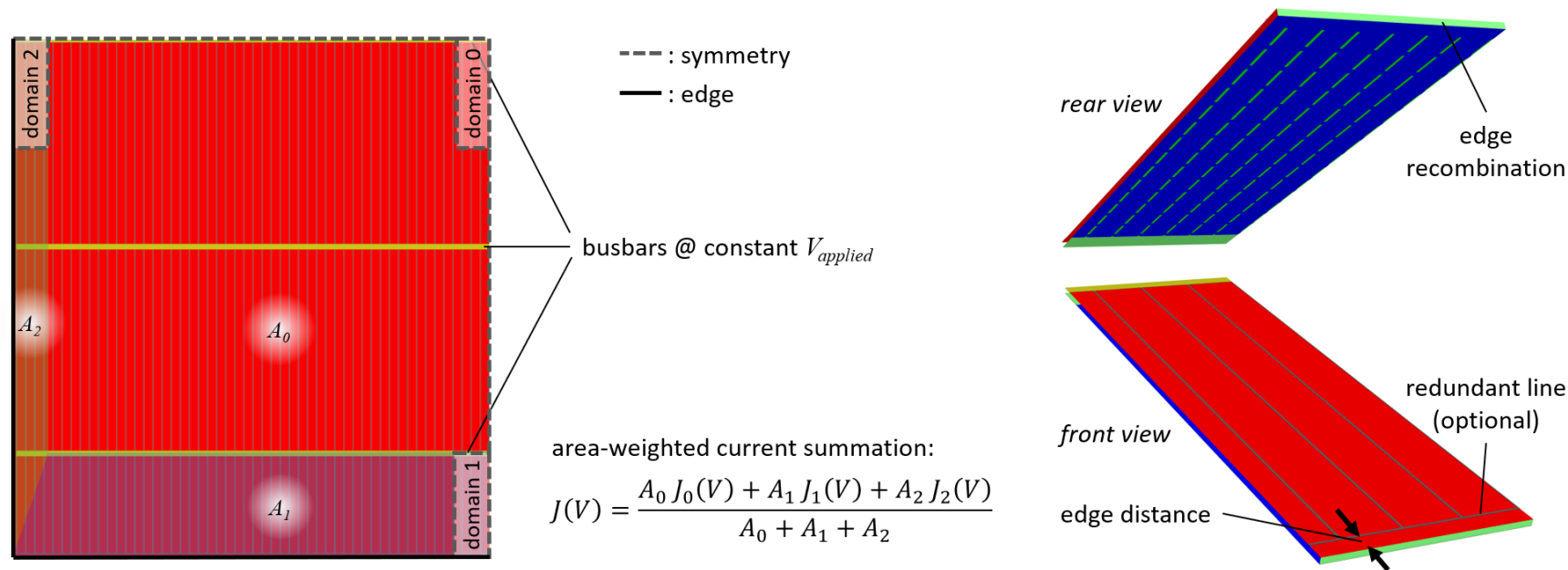
"busbar enhanced" unit cell

- Symmetry element of solar cell including half busbar pitch, accounts for
 - Different front and rear contact pitch (LCM!)
 - Busbar shading and recombination
 - Distributed finger resistance
 - Allows dashed rear contacts (not practical for full cell)



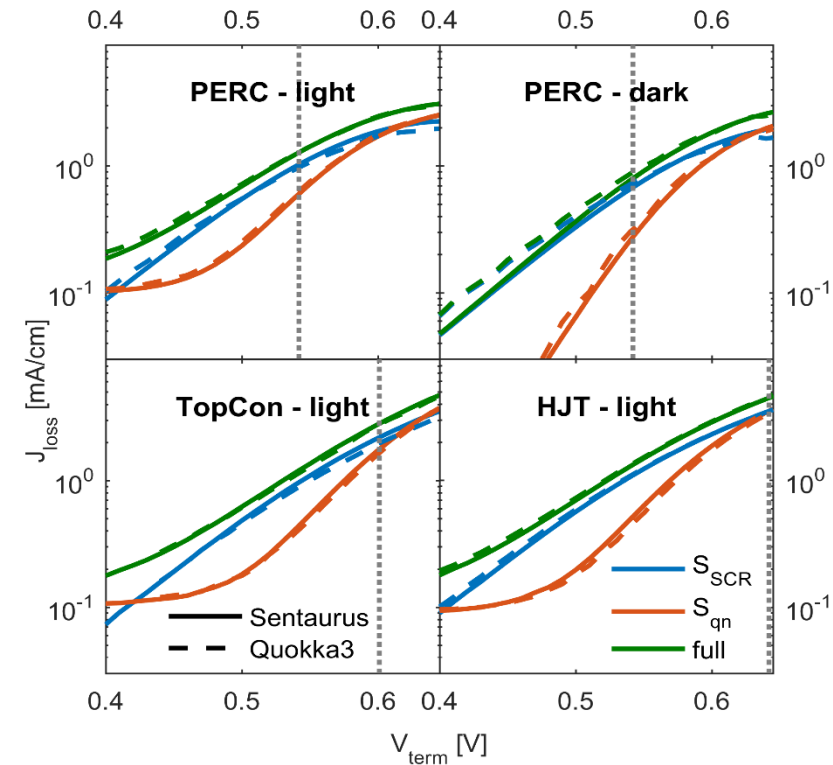
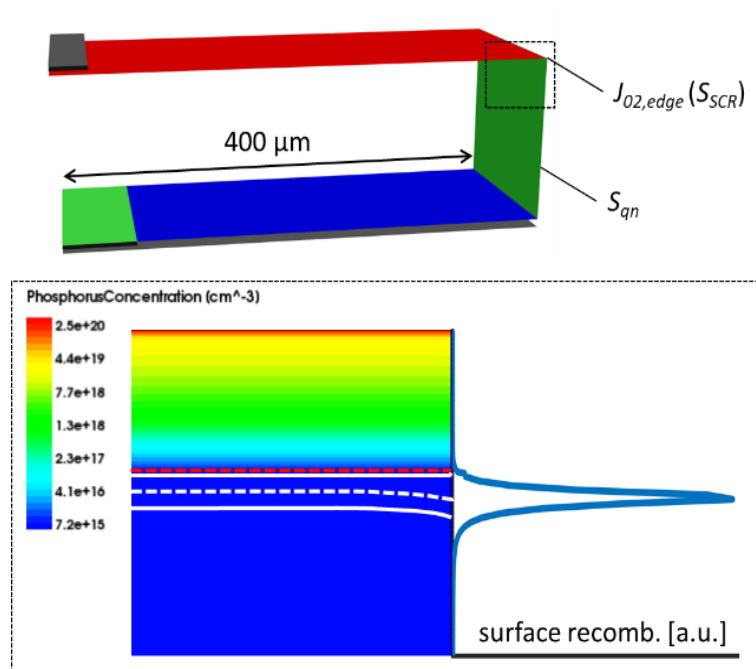
Full-cell modeling via multi-domain approach¹

- Multiple small domains represent full cell including edges with much smaller numerical mesh
- Accounting for emitter surface recombination to edge losses in a single simulation domain
- Automated in Quokka3

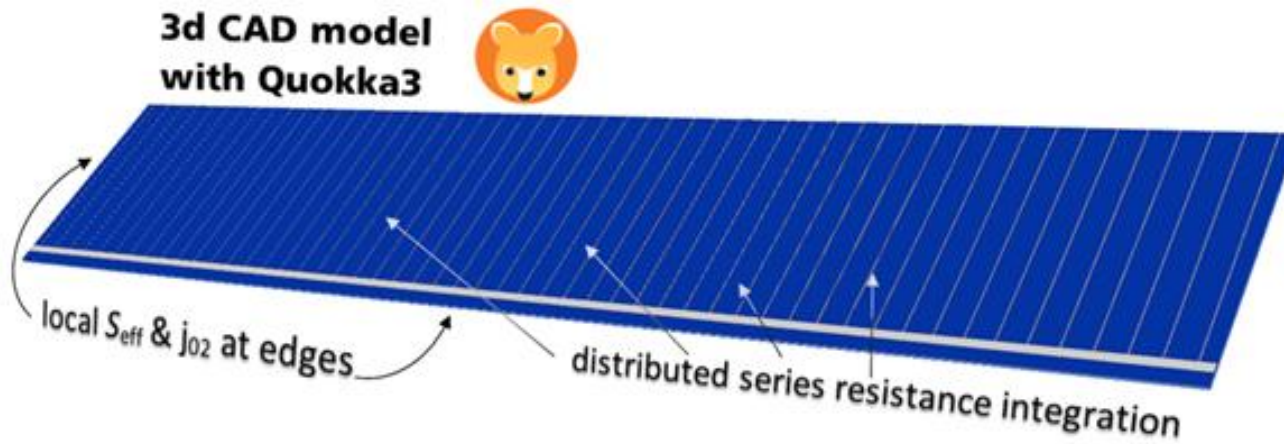


Edge recombination

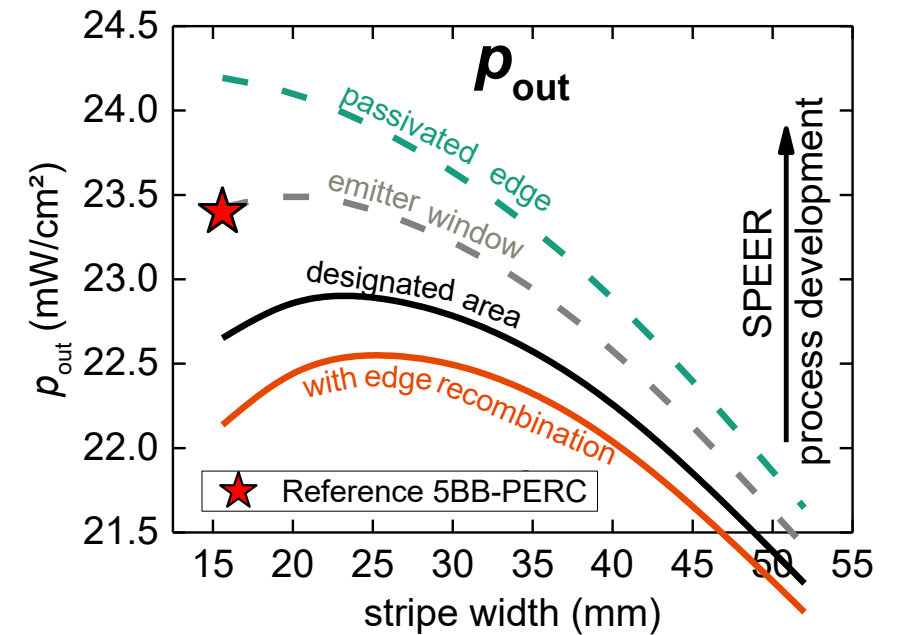
- Simulation of edge current loss both with Sentaurus Device and Quokka3
- Local $J_{02,edge}$ value of 19 nA/cm found as consistent “worst-case value”



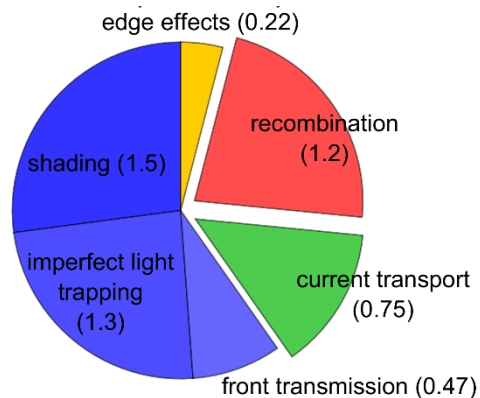
Shingle cells



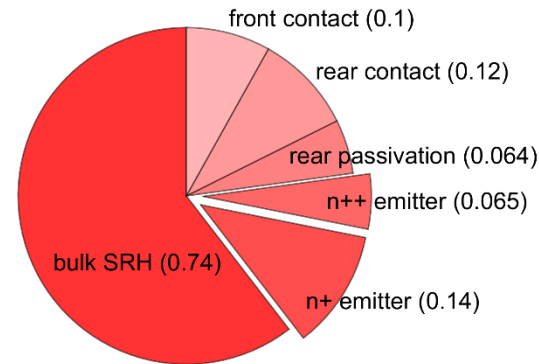
- Optimizing stripe width of shingle cell with consideration of edge effects
- Loss analysis and design rules



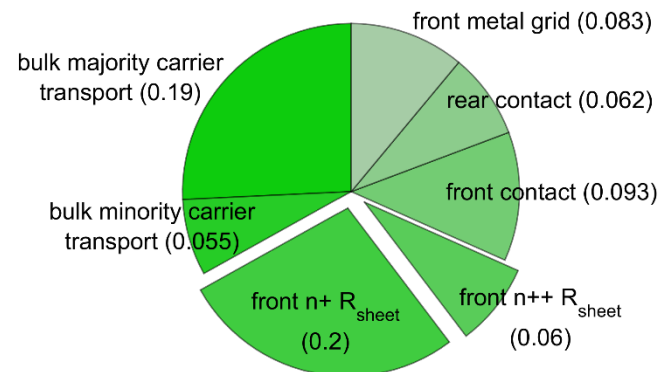
total (5.5 mW/cm²)



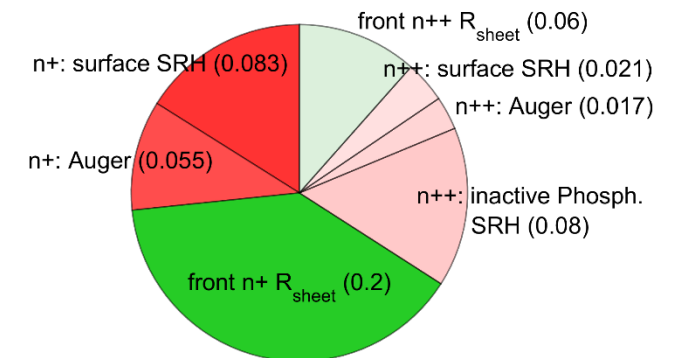
recombination (1.2 mW/cm²)



current transport (0.75 mW/cm²)



emitter (0.52 mW/cm²)



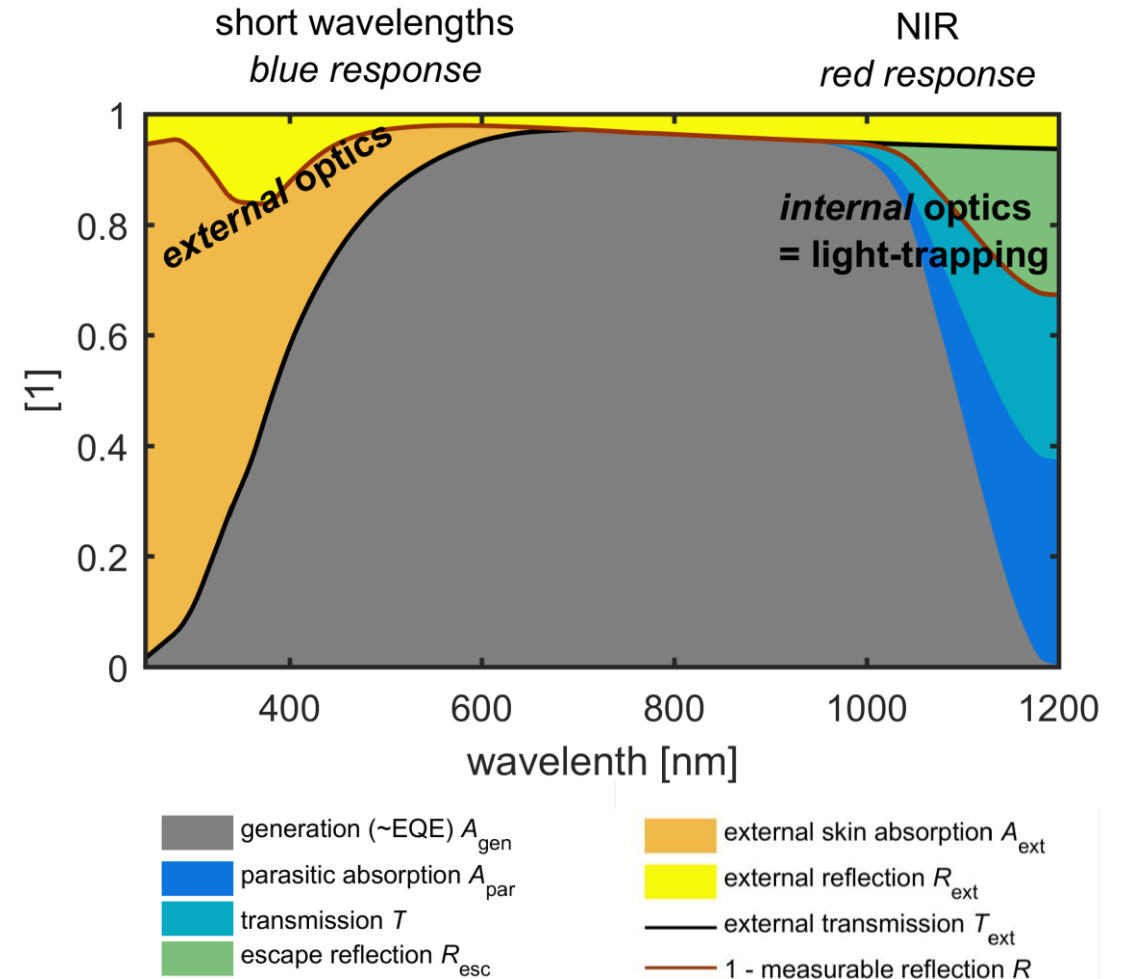
Spectrally resolved optical modeling

- **External optics**

- Defined via „ T_{ext} “: transmission of photons through the illuminated surface films into the bulk (=main absorber)
- External reflection, external parasitic absorption

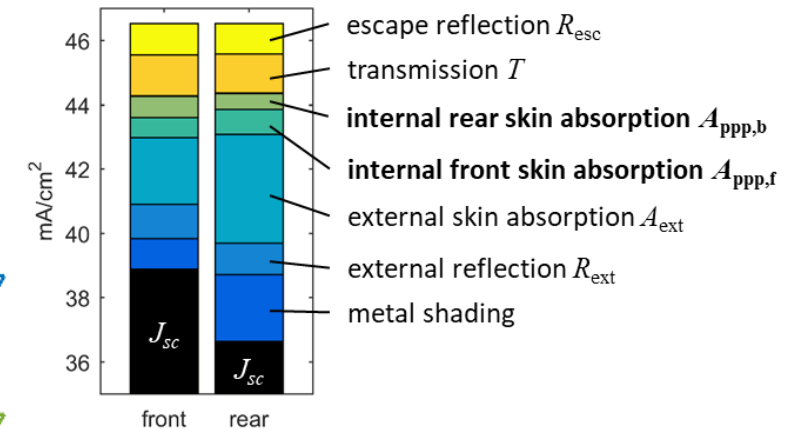
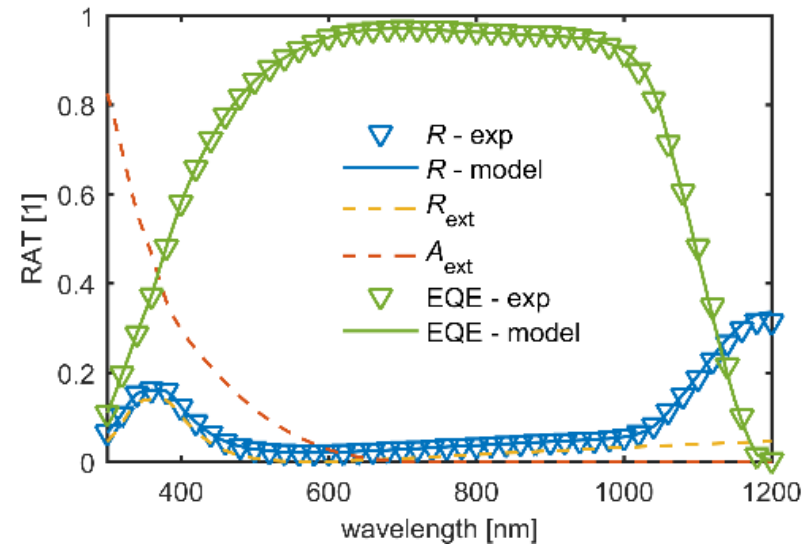
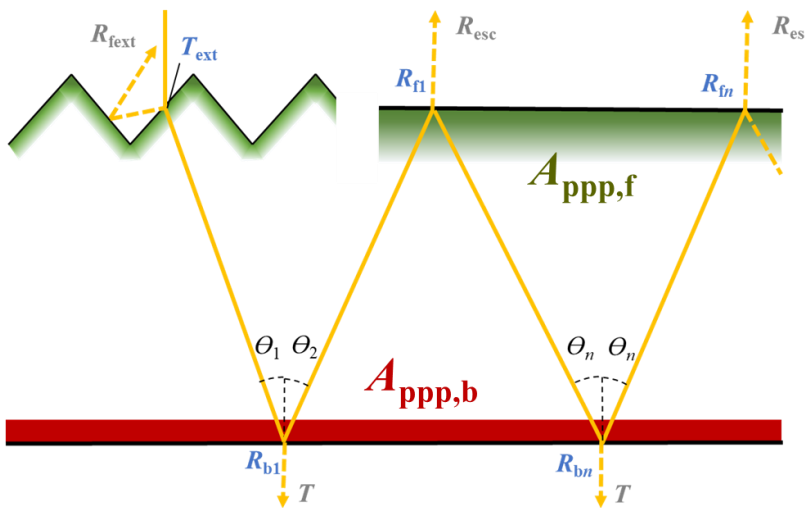
- **Internal optics** (= light trapping)

- Quantified via pathlength enhancement factor “ Z ”
 - Quokka3 implements “extended Basore model” (i.e. similar to PC1D model) to simulate light trapping¹
 - Impacts escape reflection, transmission, active absorption, NIR parasitic absorption
- Can well be calibrated to RAT measurements^{1,2} or interfaced to raytracing software
 - Well suitable for bifacial illumination



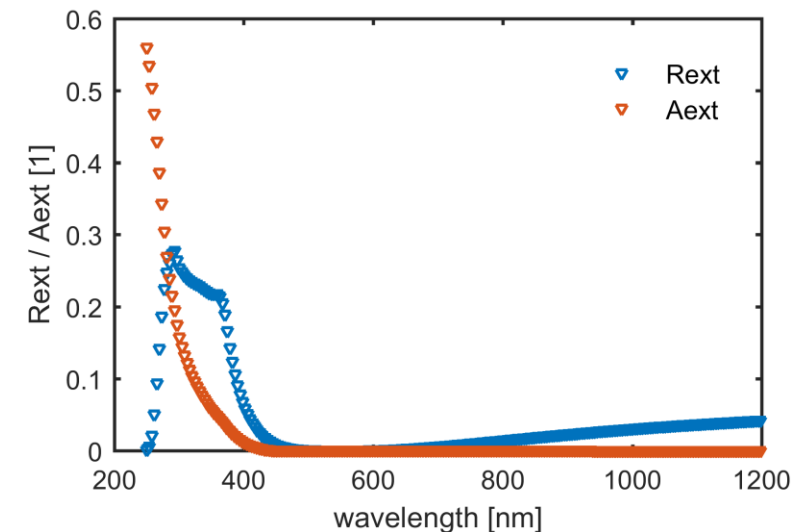
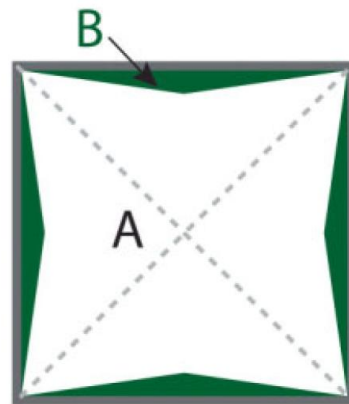
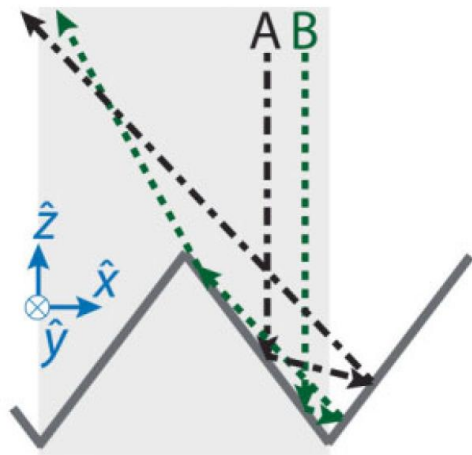
Parasitic absorption in passivating contact layers

- Extension of Basore's light-trapping model to account for parasitic absorption within skin
- Determine parasitic absorption loss in poly-Si / HJT-stack via fit to R- and T-measurement

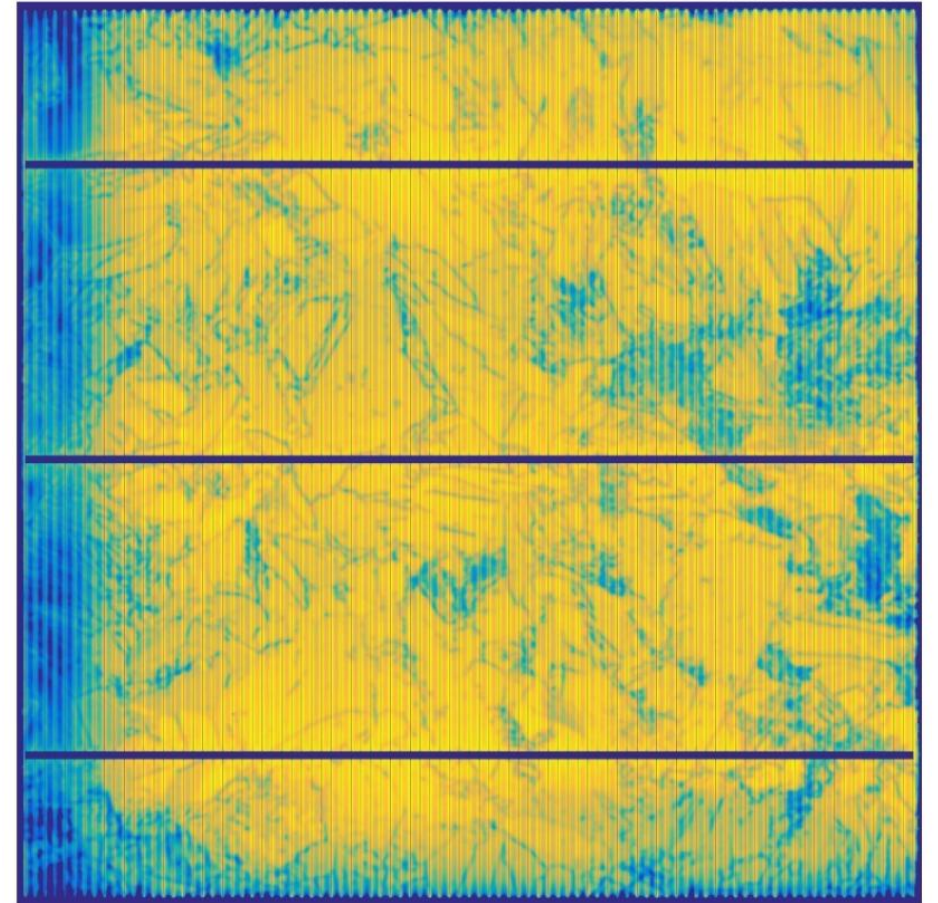


Detailed external model

- **“OPAL” algorithm¹** = simplified ray tracing + transfer matrix method (TMM), implemented in Quokka3
- Inputs: thickness + n & k of all thin films, and surface morphology (= characteristic texture angle)
- Ray tracing NOT (yet) usable for light-trapping / internal optics

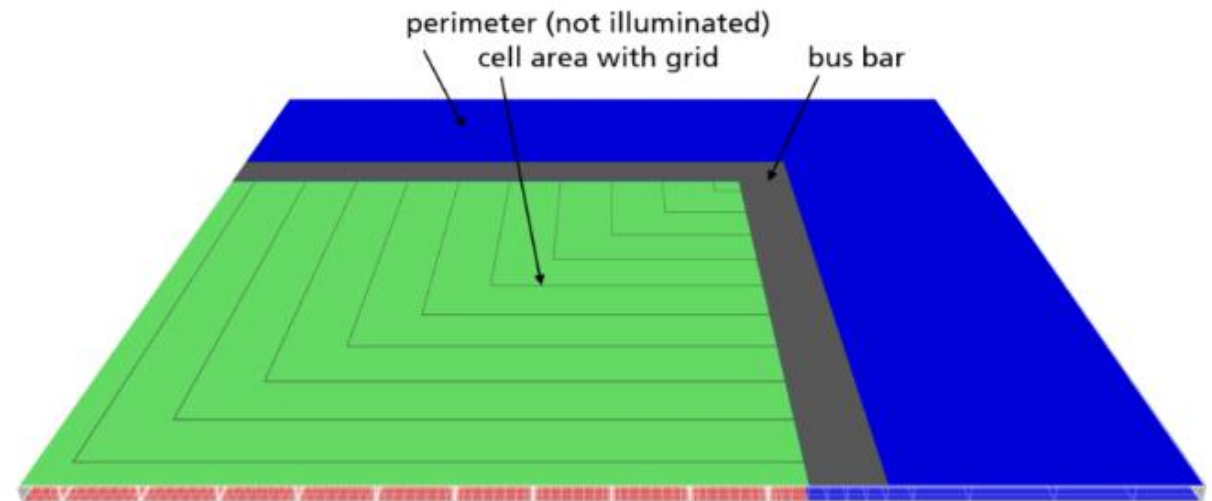
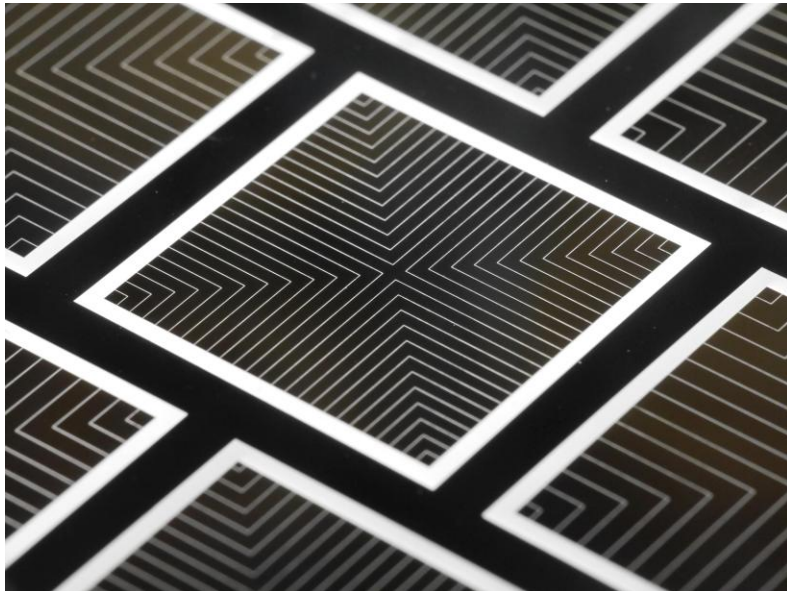


- Quokka3 routinely calculates luminescence map and spectrum from electrical solution
 - EL, PL, hyperspectral imaging
- Supports luminescence-based characterization techniques
 - E.g. contact recombination analysis¹



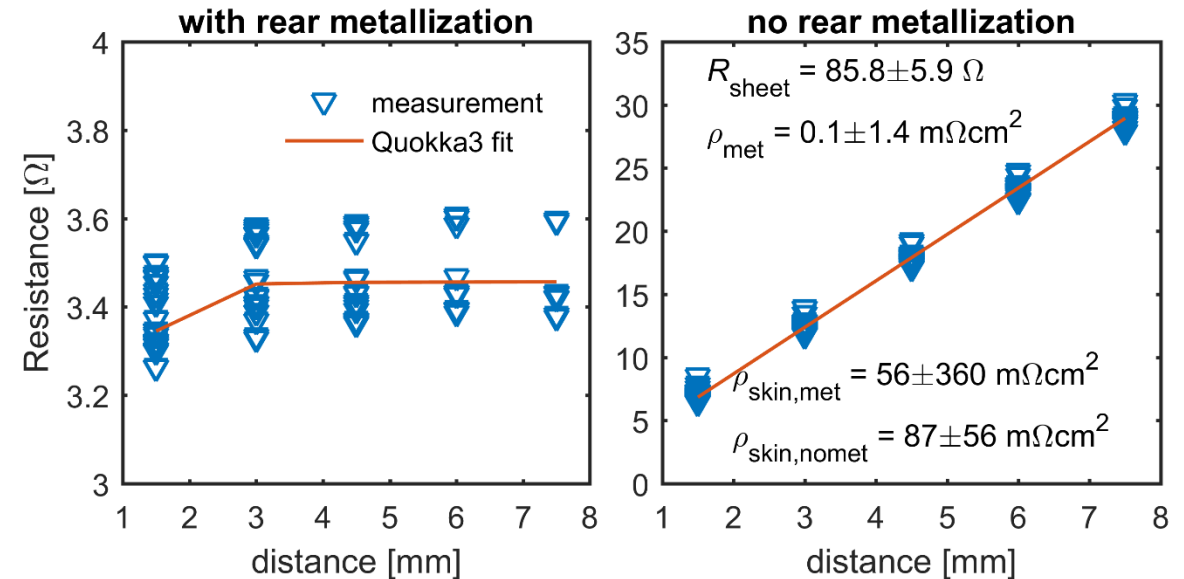
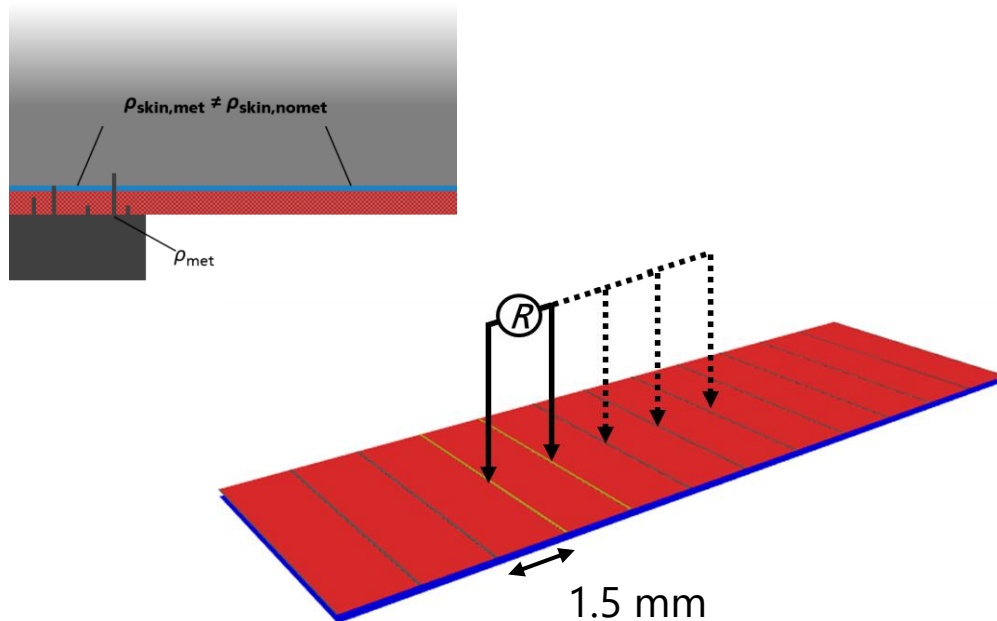
Passivating contacts – ISE TOPCon

- Quokka3 can well simulate **solar cells with passivating contacts!**
 - ISE TOPCon solar cells routinely simulated with Quokka3¹
 - Routinely used by customers for TOPCon, POLO, HJT, ...



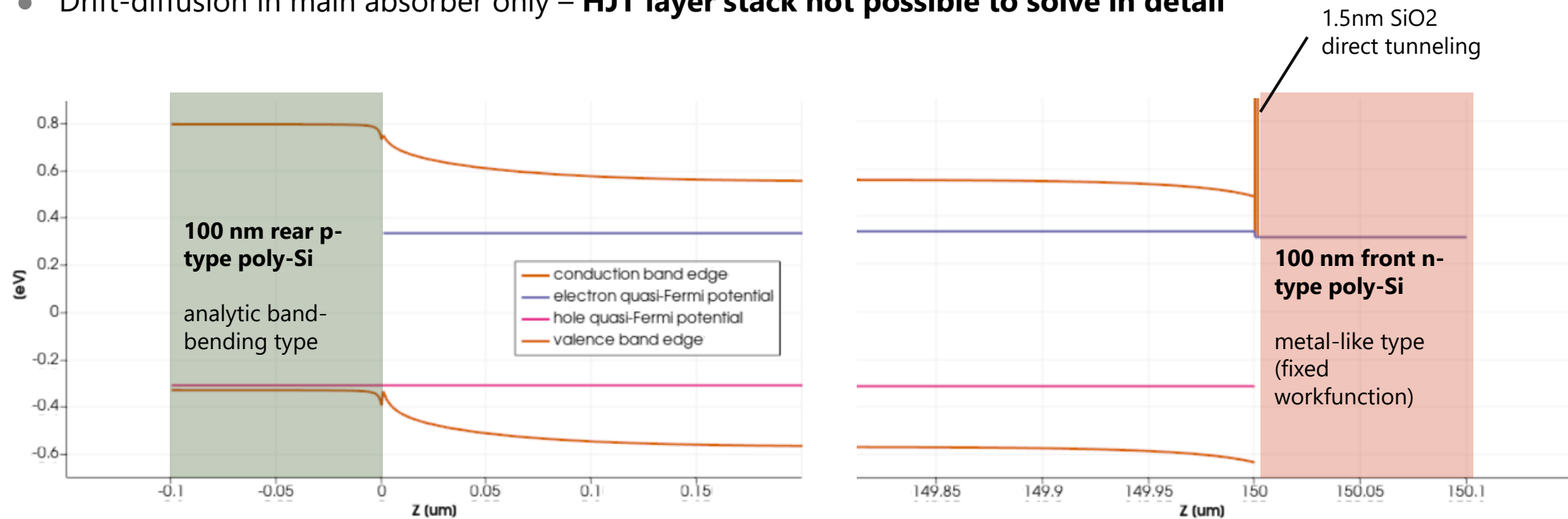
Resistive device + optimizer

- “resistive device” to simulate resistance structures, e.g. advanced TLM structures
- “biTLM”: fit 3 contact resistivities + sheet resistance to TLM measurement with and without rear metallization



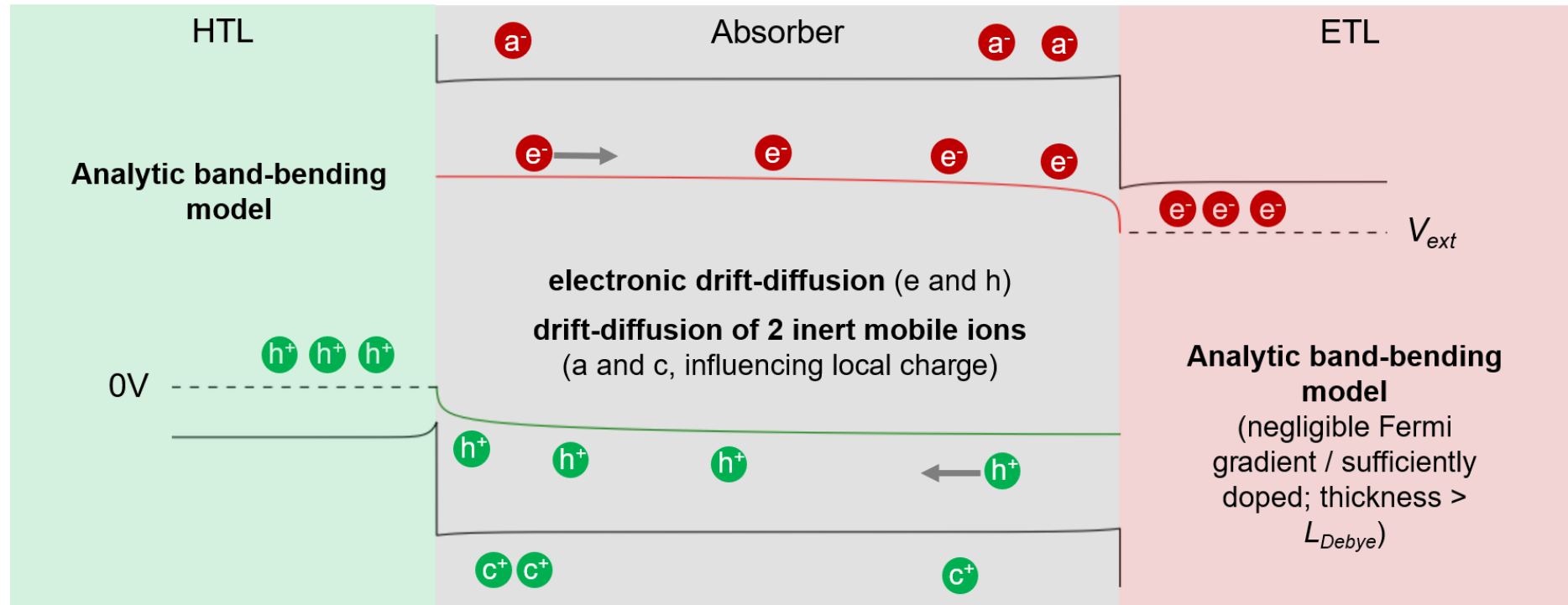
Passivating contacts - 1D detailed solver

- In 1D, Quokka3 can solve full drift-diffusion equations, and calculate band-bending effects
- Via an analytical model, band-bending within transport layers can be resolved as well
- Drift-diffusion in main absorber only – **HJT layer stack not possible to solve in detail**

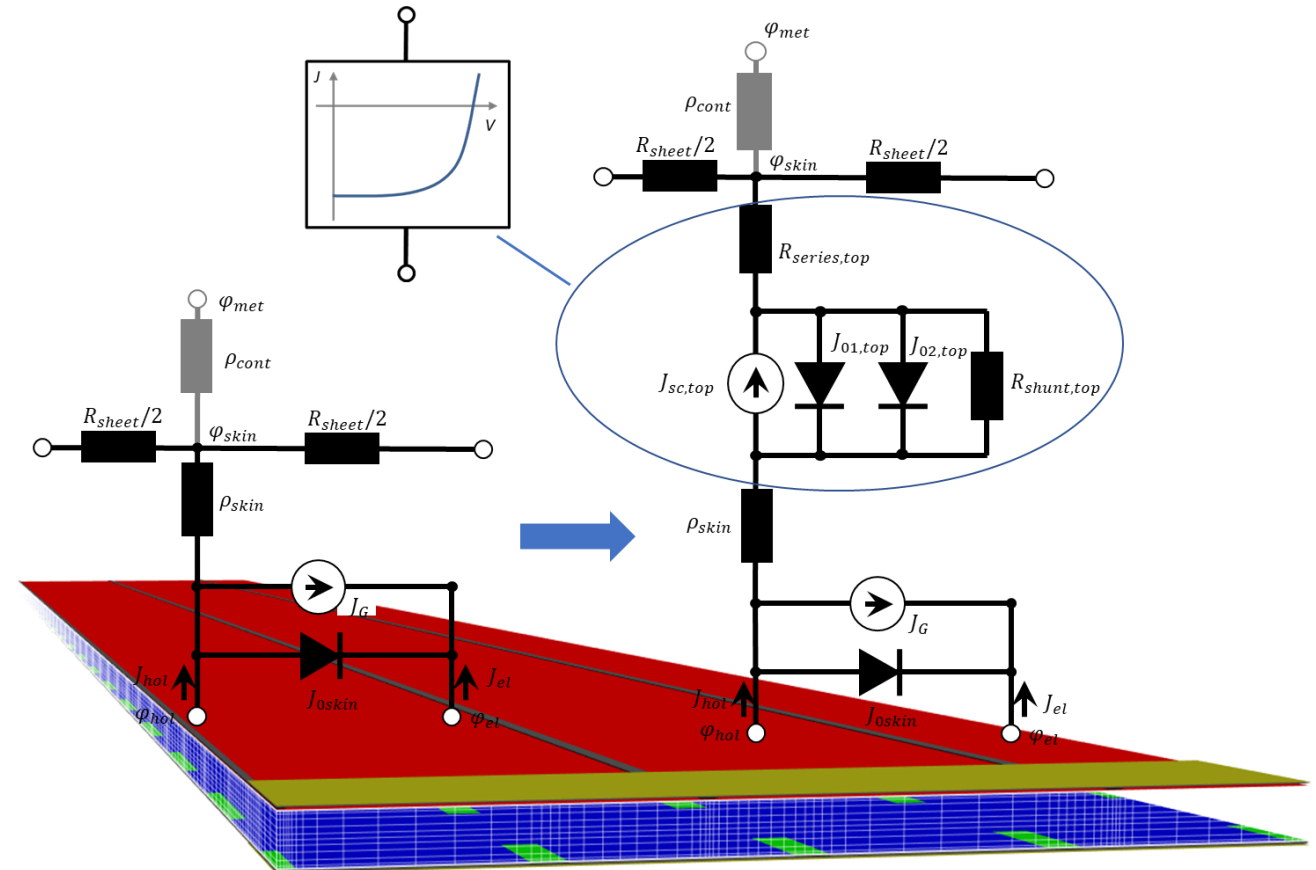


Perovskite solar cell – single junction 1D

- Electronic-**ionic** drift-diffusion; **transient** + steady-state
- Simplified transport layer models (no drift-diffusion in transport layers)



- Subcell can be defined as an equivalent circuit model within a skin
- Enables large-area 3D tandem modeling, when JV + EQE of top cell is known
- Grid optimization
- Edge effects
- Loss analysis
- Inhomogeneities
- ...



KAUST PVK-Si tandem

- Detailed optical model with all film's thickness + n&k values
- 3D shunt-quenching simulations

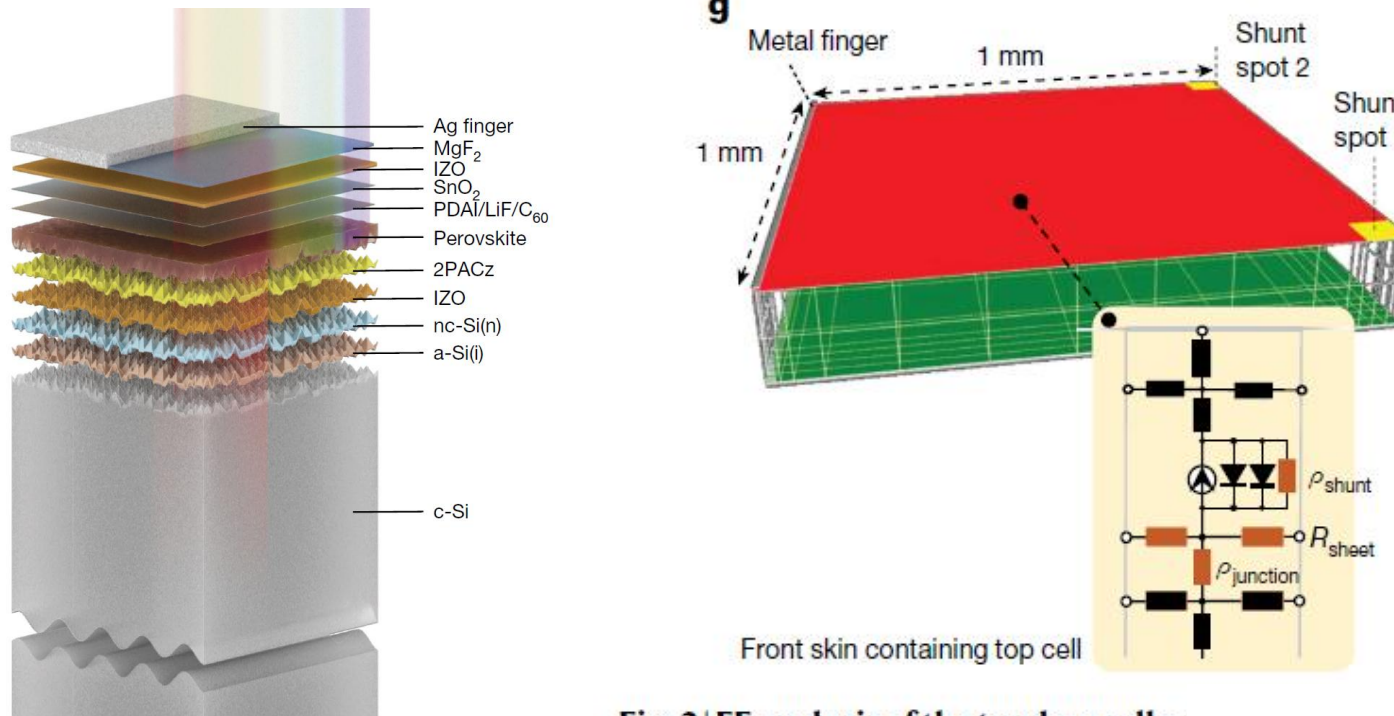
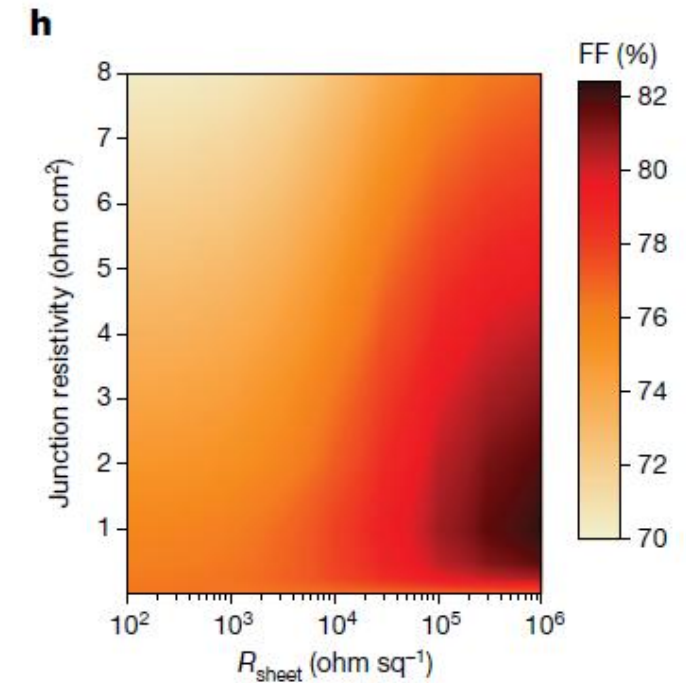
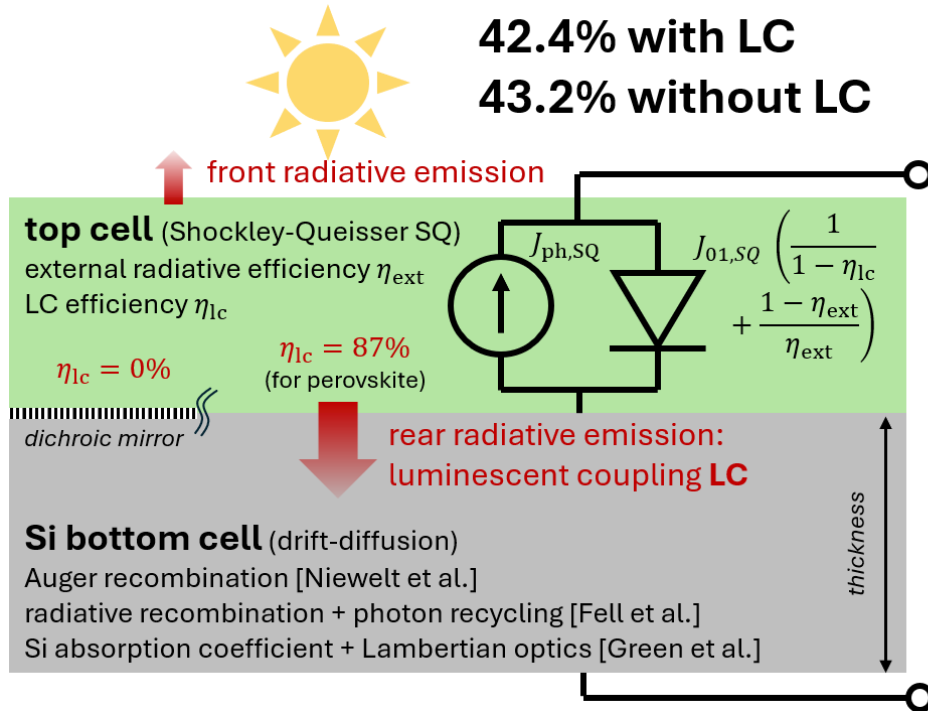


Fig. 2 | FF analysis of the tandem cells.



Tandem: Shockley-Queisser topcell + luminescent coupling

- Topcell can easily be defined by radiative limit (bandgap) + ERE
- Luminescence emission + coupling from topcell EQE and reciprocity



front emission
photon flux:

$$\phi_{\text{front}} = \int \frac{2\pi E^2}{h^3 c^2} \frac{\text{EQE}(E)}{\exp\left(\frac{E - qV}{kT} - 1\right)} dE$$

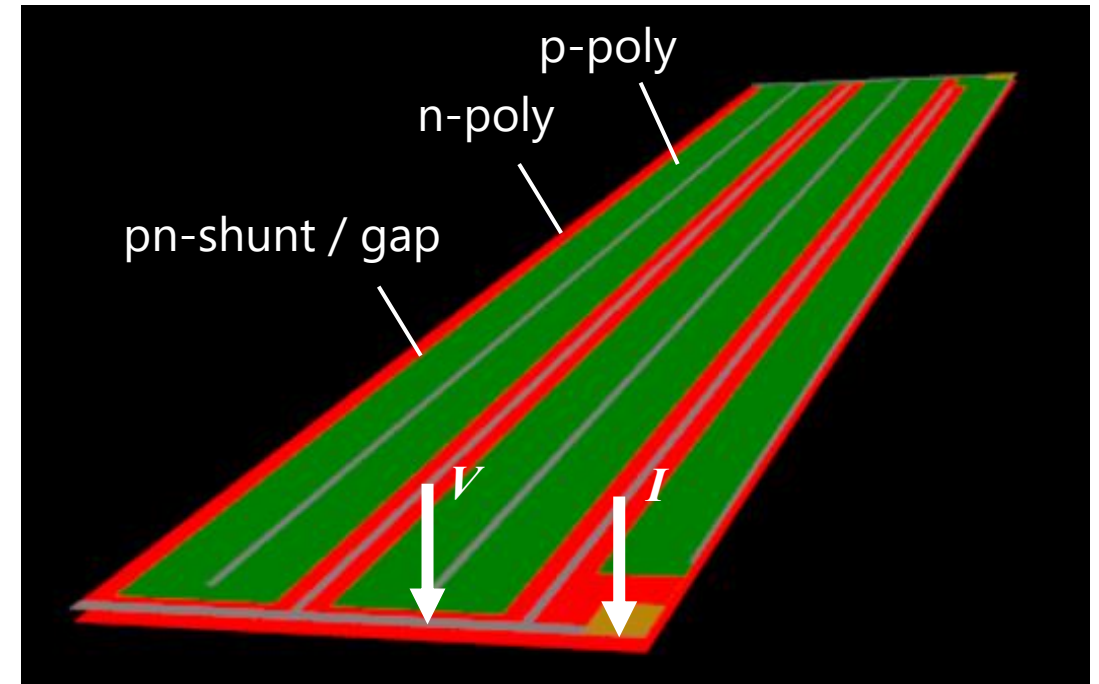
coupling efficiency:

$$\eta_{\text{lc}} = \frac{\phi_{\text{rear}}}{\phi_{\text{front}} + \phi_{\text{rear}}}$$



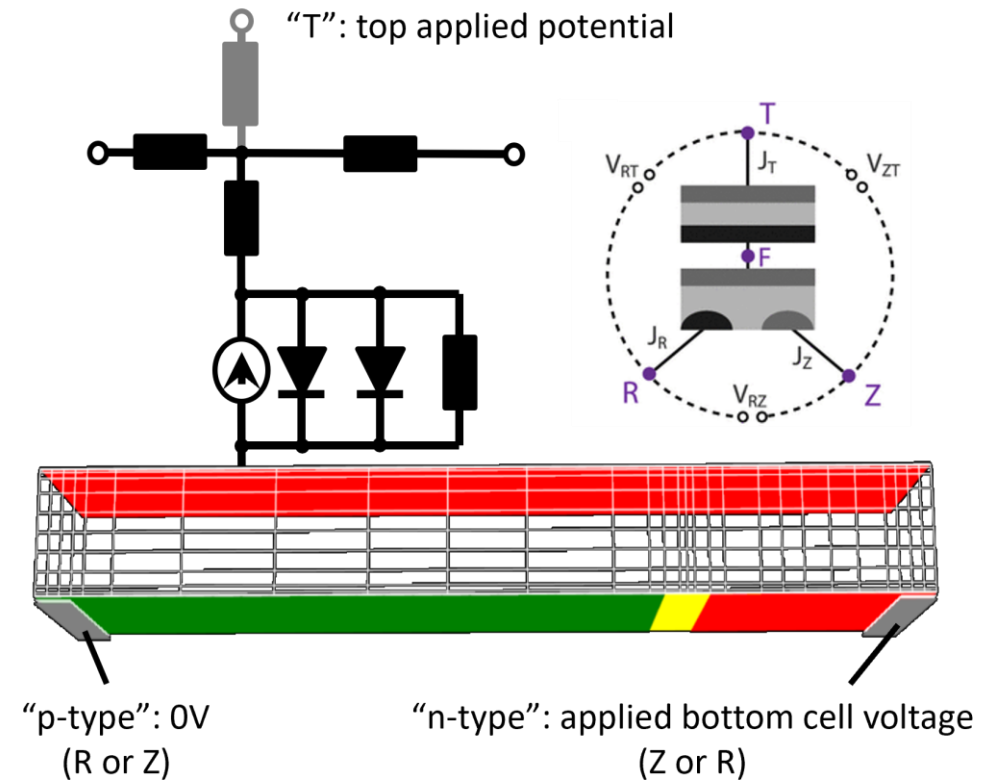
IBC syntax example: TBC cell

- Poly-Si properties (doping / thickness)
 - Parasitic absorption
 - Sheet and contact resistance, recombination
 - Poly-finger
- PN-shunt / gap properties
- Investigate / optimize geometry
 - N-width / P-width
 - Finger pitch, finger resistance
 - Solder-pad size
- Investigate edge effects (recombination, transport)
- Represent IV-contacting (FF effects)



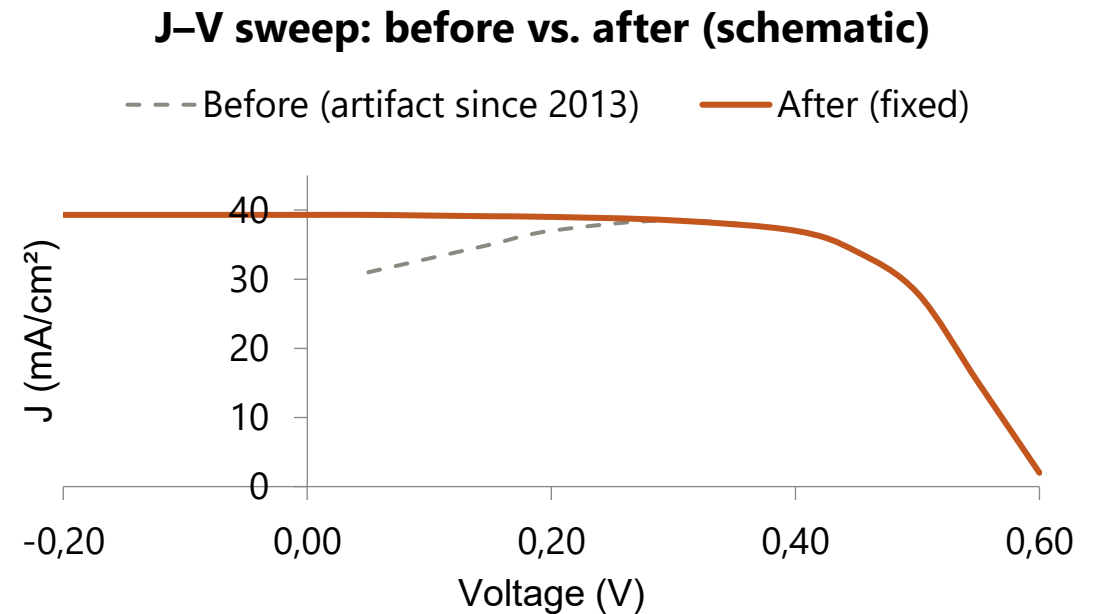
3-terminal tandem

- IBC + topcell skin = 3T tandem
- Voltage-match option
- Shared current path physics



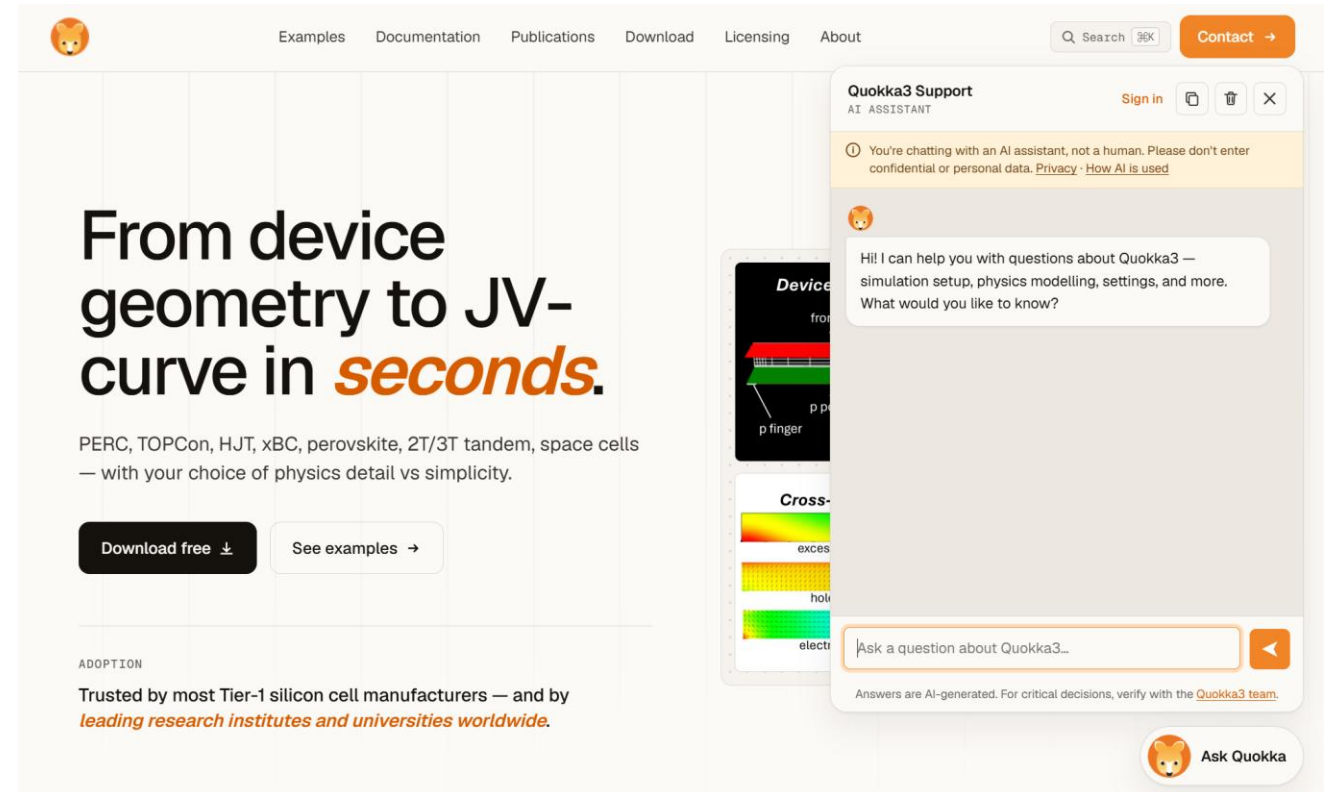
Since version 3: small / reverse bias working

- For 13 years I accepted that the missing pn-junction / space-charge-region (SCR) in the skin model (= conductive boundary model) does not work at short-circuit
- Current was wrong – JV sweep algo stopped at flat part (sufficiently accurate)
- Wrong: it “just” needed the correct physical-numerical implementation
- Enabler for reverse breakdown physics (future update)



Soon: AI integration

- First step: chatbot on new website
 - Backed by substantial Quokka3 and solar cell modeling knowledge base (support emails)
- Next step: MCP server tools
 - Talk to your AI which is smartened by knowledge base, creates settingsfiles, runs simulations, and plots results



- **Fully committed** to provide the PV community with the best solar cell simulation tool for foreseeable future (private business)
- **Business going well**, > 30 paying companies and research institutes, including most Tier-1 Chinese solar cell manufacturers
- Next steps
 - AI integration
 - Reverse breakdown
 - Drift-diffusion in layers
 - Yield
 - ...?

