Charge transport in perovskites solar cells: modeling, analysis and simulations

Weierstrass Institute Berlin

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NUMSEMIC
Numerical Methods for
Innovative Semiconductor Devices

joint work with

Dilara Abdel (WIAS), Claire Chainais-Hillairet (Inria Lille), Maxime Herda (Inria Lille)

Inria-ECDF Partnership Kick-Off Workshop
6 June 2024

Leibniz Association MATH+ Inria EINSTEIN CENTER Digital Future

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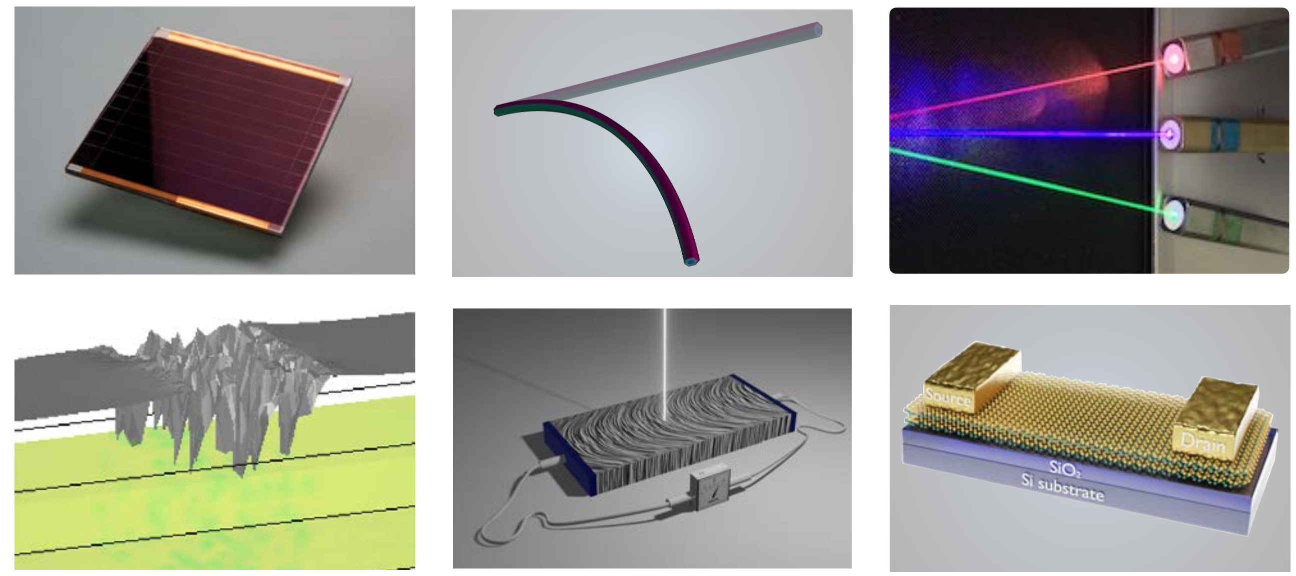
Numerical Methods for Innovative Semiconductor Devices

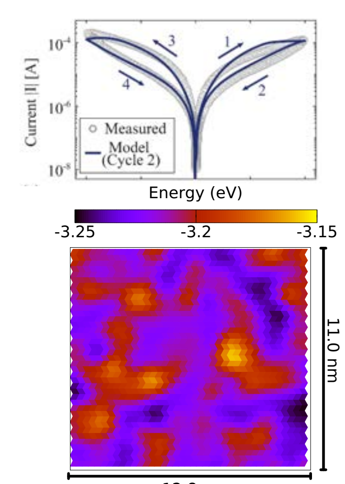
Applications

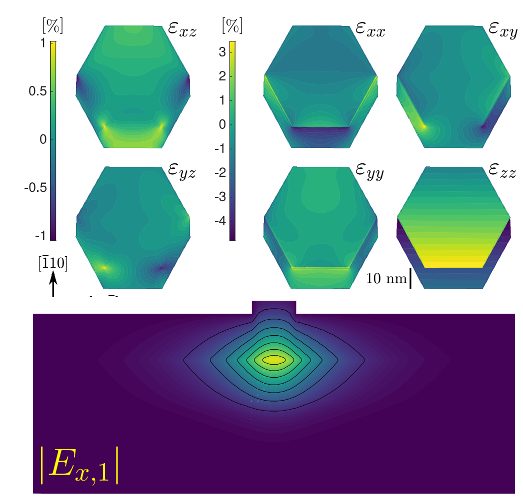
- perovskites
- quantum wells
- lasers
- bending nanowires
- crystal quality
- 2D TMDC memristors



Mathematical topics

- charge transport ("van Roosbroeck system")
- finite strain elasticity models
- Helmholtz equation
- meshfree, multiscale, data-driven methods
- hysteresis, inverse problems, LLT





Collaborations

- 15 partners from mathematics, physics and engineering

  Inria/U Lille, Oxford, U Florence, U Catania, TU Vienna, U Florence, U Pisa,
  TU Ilmenau, U Rosario, Tyndall Institute, PDI, IHP, ZIB, HZB, IKZ

Existing collaboration

Weierstrass Institute for Applied Analysis and Stochastics

Patricio Farrell

Dilara Abdel

Inria Université de Lille

Claire Chainais-Hillairet

Maxime Herda

Existing collaboration

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Claire Chainais-Hillairet


Maxime Herda


Marianne Bessemoulin-Chatard (now Nantes)


Benoît Gaudeul (now U Paris Saclay)


Julien Moatti (now TU Vienna)

Existing collaboration

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Julien Moatti (now TU Vienna)

- fruitful collaborations: theory driven by applications
- first joint publication by Chainais-Hillairet & Fuhrmann in 2012
- several research visits both ways

Solar cells based on...

Silicon

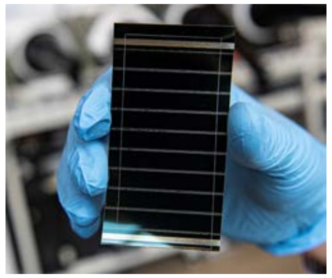
- relatively cheap
- last long (25 years)
- 70,600 MW installed
- ~50 nuclear power plants



Lason *Dreamstime.com*

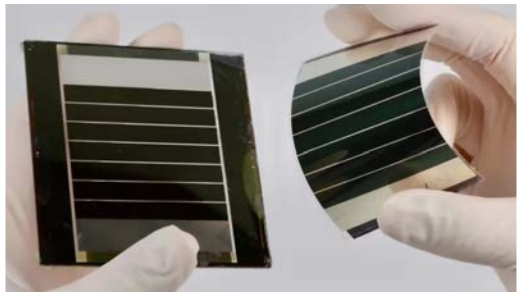
Perovskites

- relatively cheap
- new, still unstable
- but in the lab more efficient



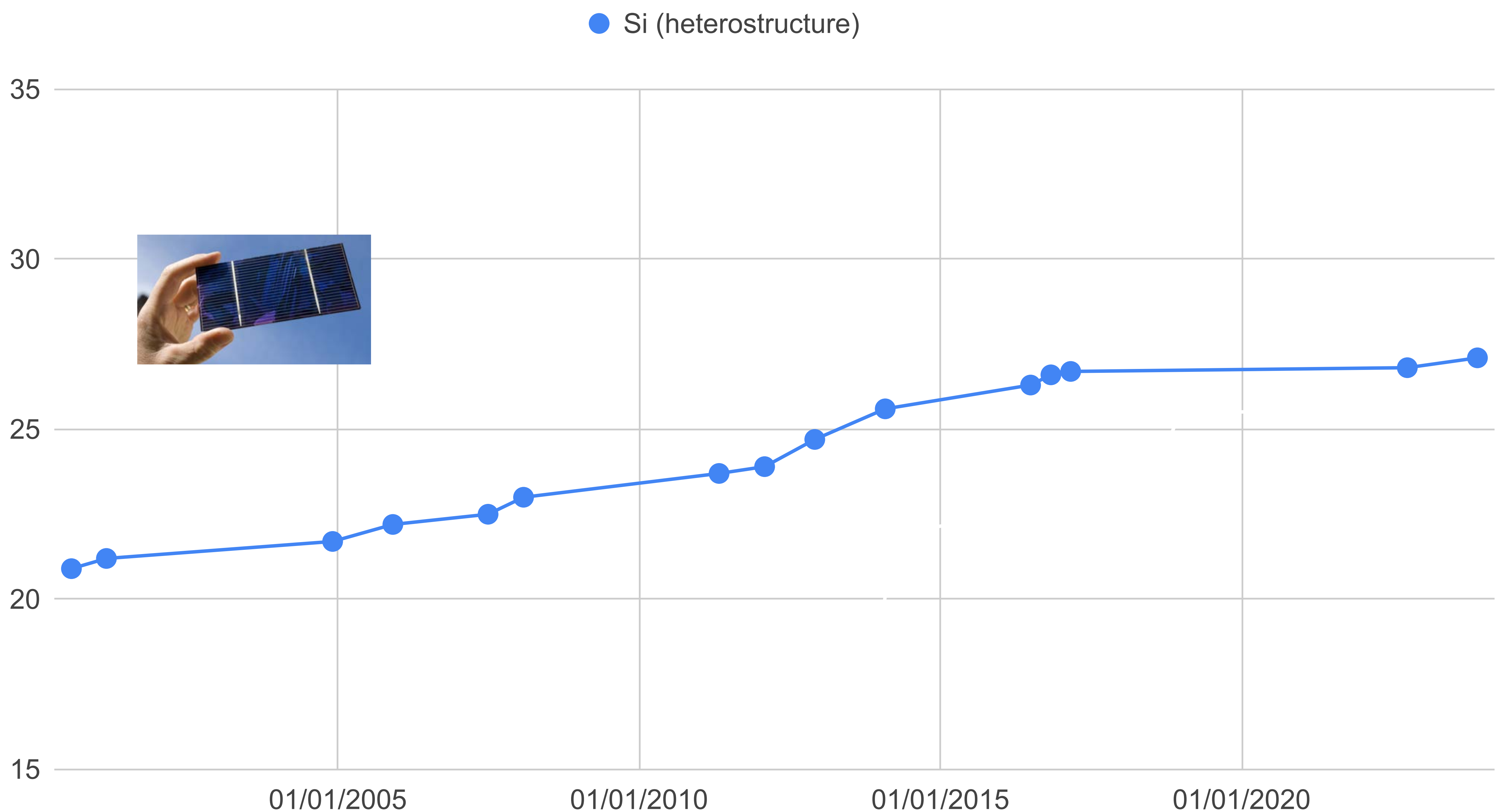
Dennis Schroeder

E. Kymakis

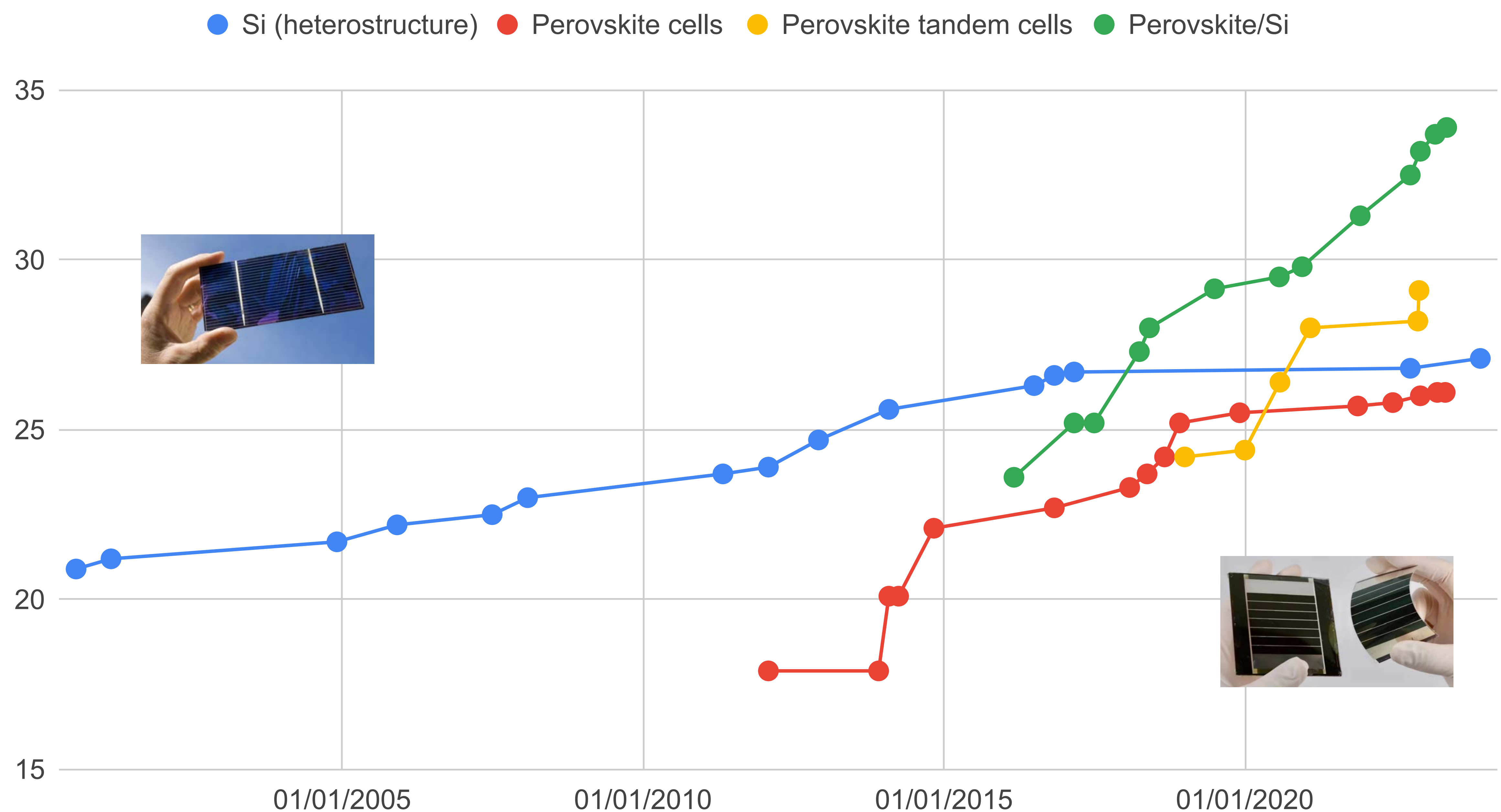


Kyoto University

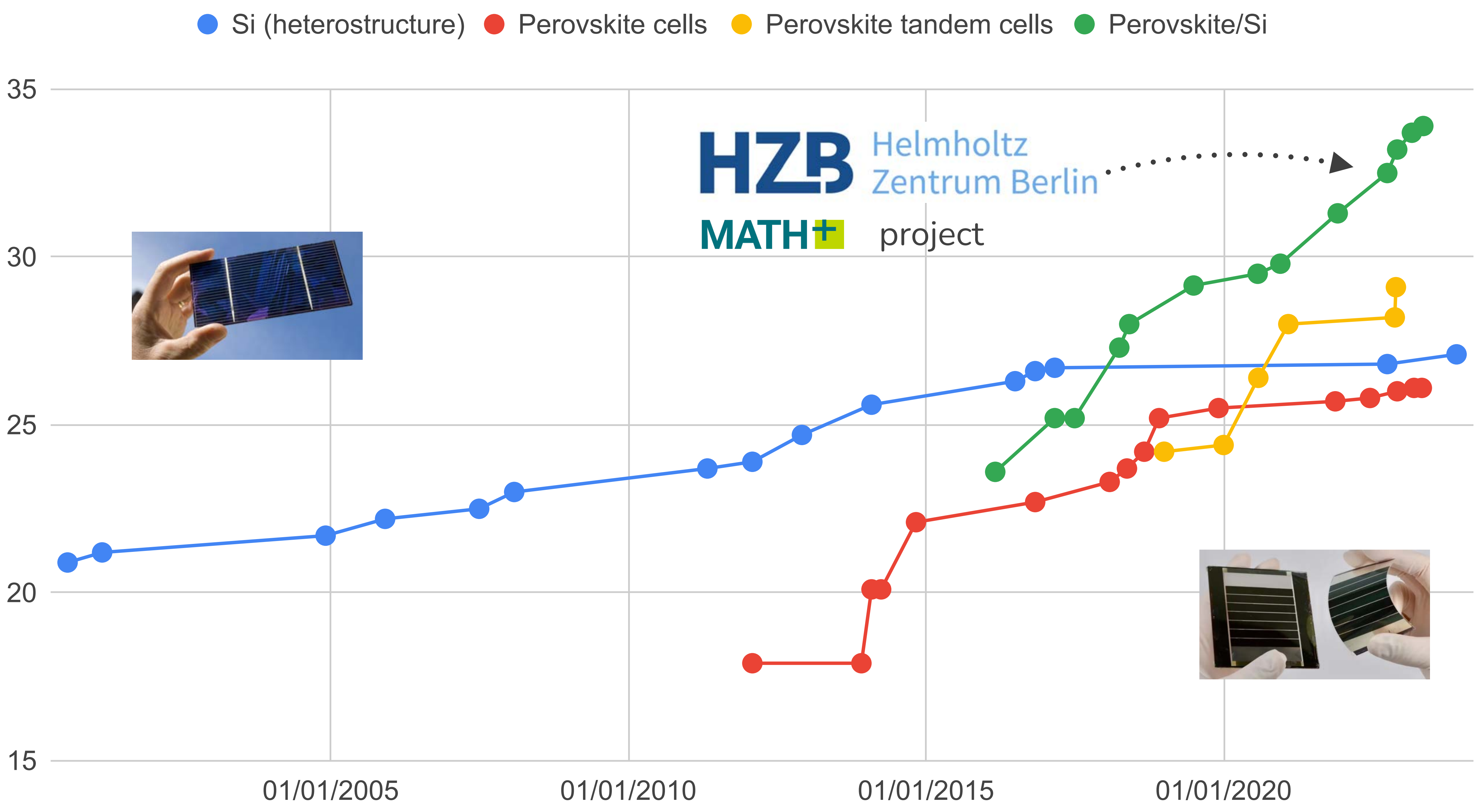
World-record efficiency [%]



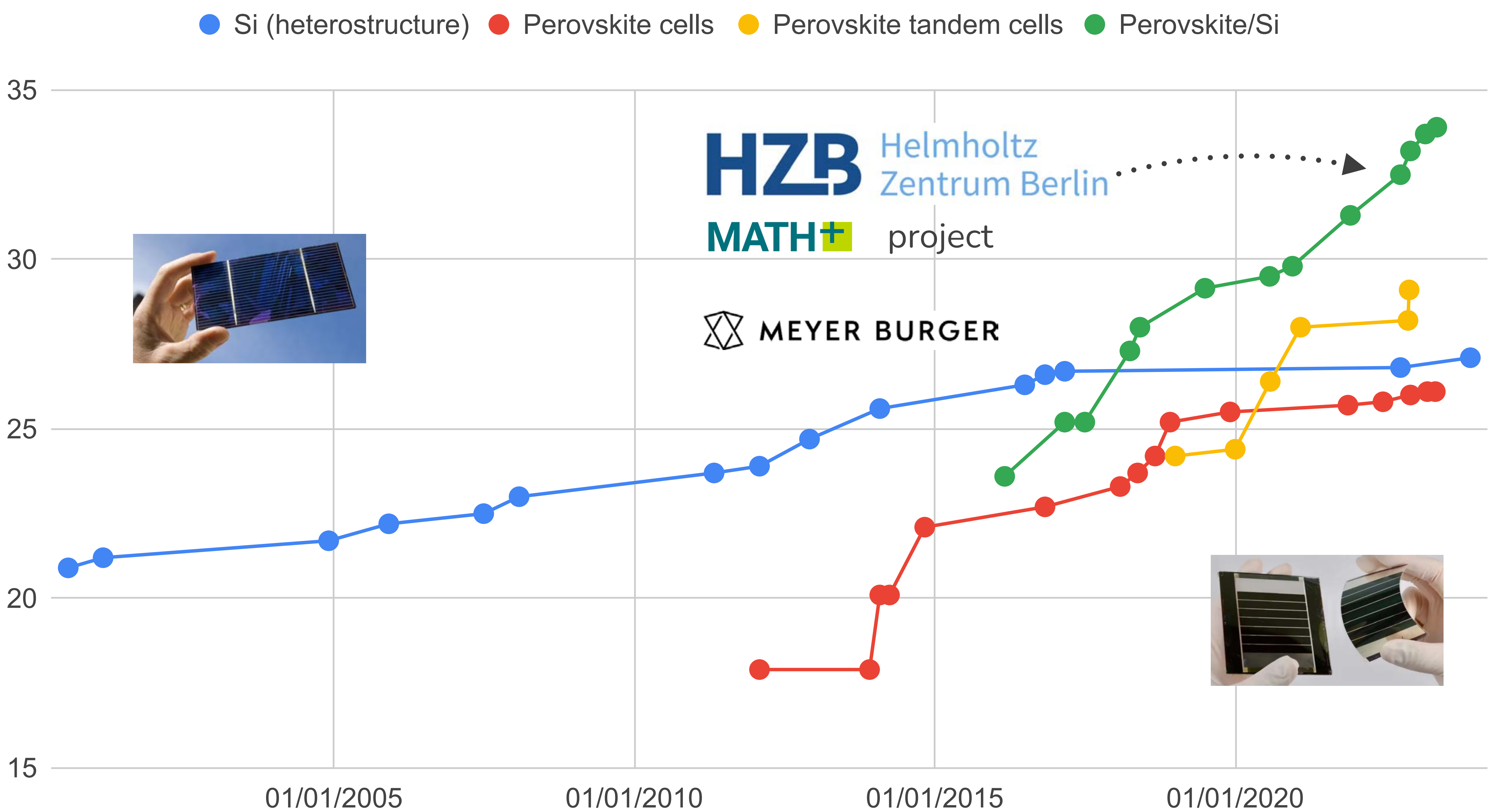
World-record efficiency [%]



World-record efficiency [%]



World-record efficiency [%]

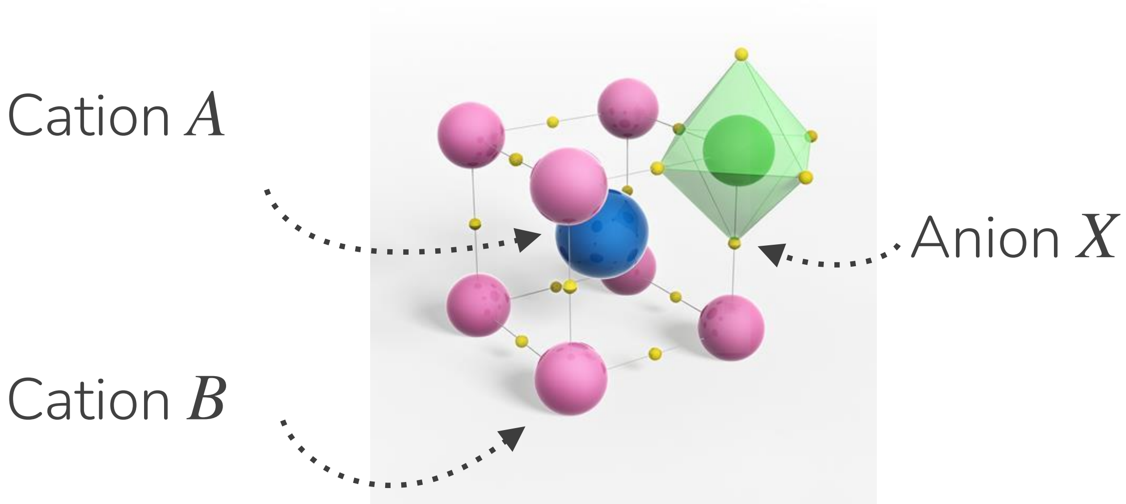


Perovskites

Generic material structure

$$ABX_3$$

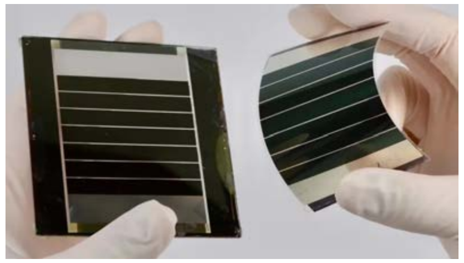
e.g. MAPI $(CH_3NH_3)^{+}Pb^{2+}(X^{-})_3$



Russian mineralogist Perovski

Applications

- solar cells
- photobatteries
- magnets
- lasers
- data storage



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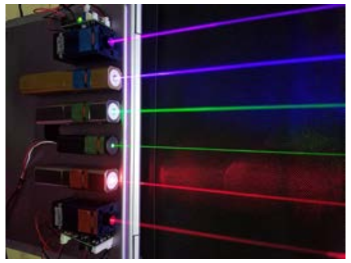
computer generated



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Thor Balkhed

Jumia

How to turn this problem into mathematics?

Modeling [1)]

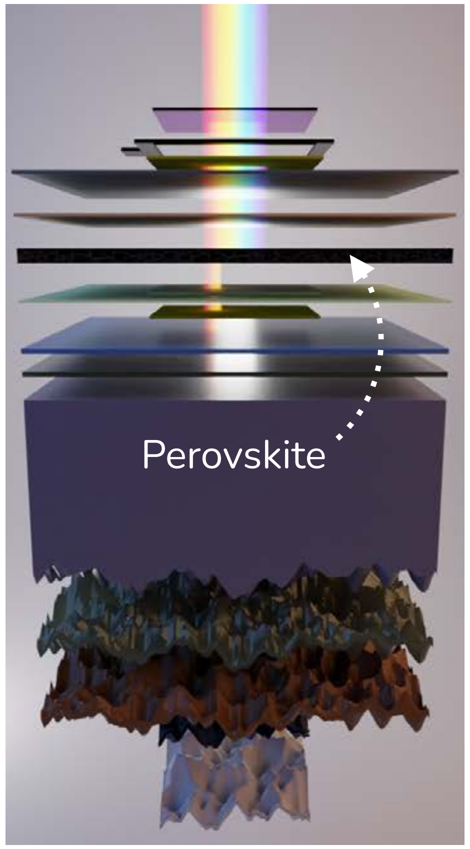
- charge transport
- drift-diffusion PDE

Analysis [2), 3)]

- existence of sol. for PDE
- two-point flux FVM
- existence of sol. for FVM

Simulation [2), 4)]

- different flux models

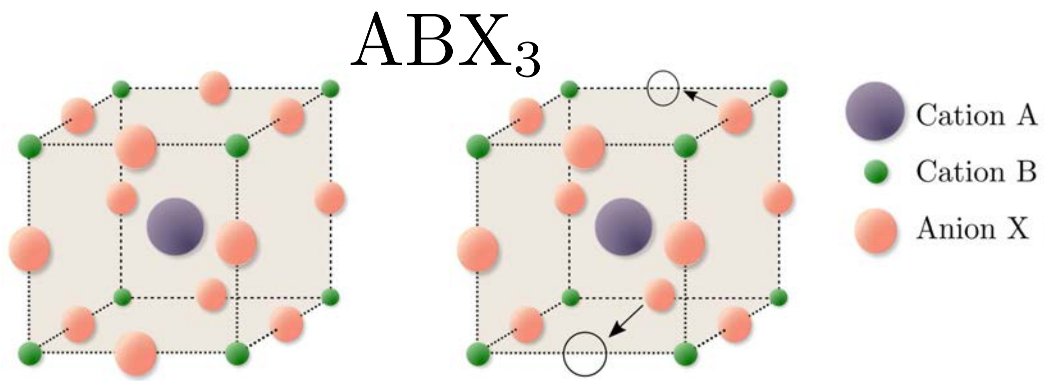


1) D. Abdel, P. Vagner, J. Fuhrmann, P. Farrell. *Modelling charge transport in perovskite solar cells: Potential-based and limiting ion depletion*. Electrochimica Acta, 390: 138696, 2021.
2) D. Abdel, C. Chainais-Hillairet, P. Farrell, M. Herda. *Numerical analysis of a finite volume scheme for charge transport in perovskite solar cells*. IMA Journal of Numerical Analysis, 2023
3) D. Abdel, A Glitzky, M. Liero. *Analysis of a drift-diffusion model for perovskite solar cells.* Accepted for publication in DCDS-B, 2024.
4) D. Abdel, N. Courtier, P. Farrell. *Volume exclusion effects in perovskite charge transport modeling*. Optical and Quantum Electronics, 55(884), 2023.

Modeling perovskite solar cells

Ion movement

- due to Schottky defects ions migrate
- ions move 10/15 orders more slowly

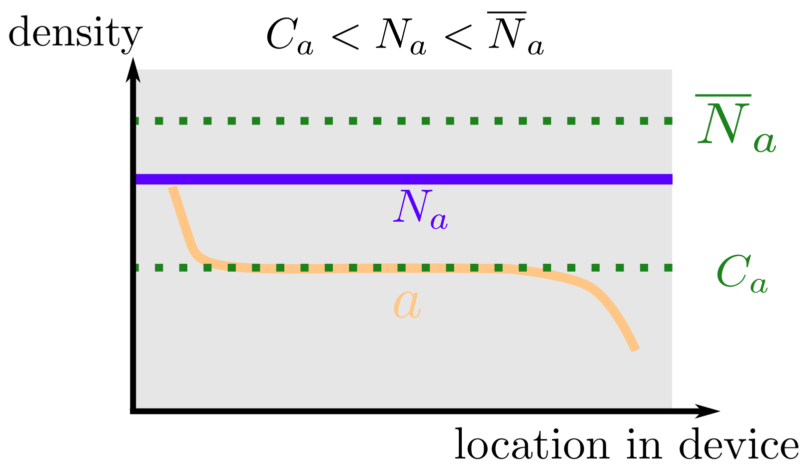


Potentials vs densities

- electrostatic/qF potentials of same order
- densities may jump a hetero interfaces
- gradient structure

Volume exclusion

- ions significantly bigger than electrons/holes
- ions cannot deplete without destroying the crystal



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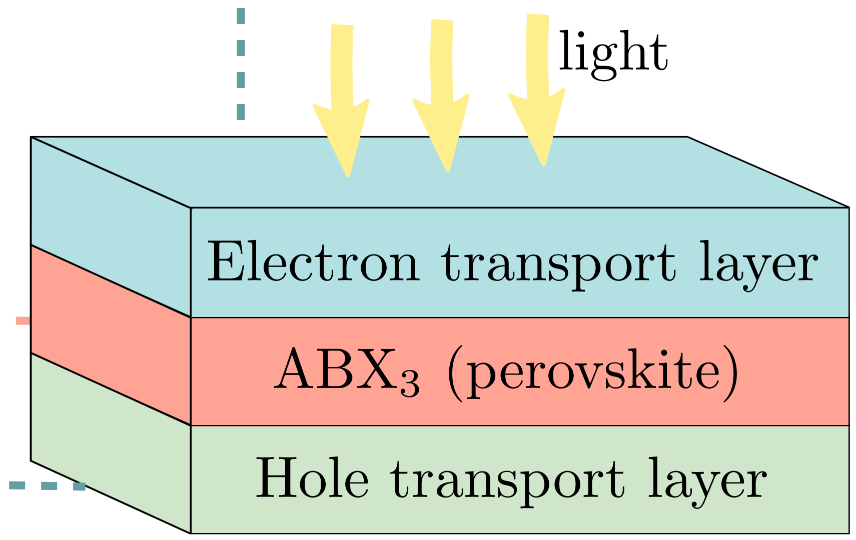
Drift-diffusion model

Transport layers

$$-\nabla \cdot (\varepsilon_s \nabla \psi) = q\,\big(C + p - n\big) \qquad \text{Poisson}$$

$$q\partial_t n - \nabla \cdot \mathbf{j}_n = q(G - R),$$
$$q\partial_t p + \nabla \cdot \mathbf{j}_p = q(G - R), \qquad \text{Cont. equations}$$

+ Dirichlet bc & ic



Perovskite layer

$$-\nabla \cdot (\varepsilon_s \nabla \psi) = q\,\big(C + p - n + a\big) \qquad \text{Poisson}$$

$$q\partial_t n - \nabla \cdot \mathbf{j}_n = q(G - R),$$
$$q\partial_t p + \nabla \cdot \mathbf{j}_p = q(G - R), \qquad \text{Cont. equations}$$
$$q\partial_t a + \nabla \cdot \mathbf{j}_a = 0$$

+ hom. Neumann bc & ic

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Drift-diffusion model

Transport layers

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$$q\partial_t n - \nabla \cdot \mathbf{j}_n = q(G - R),$$
$$q\partial_t p + \nabla \cdot \mathbf{j}_p = q(G - R), \qquad \text{Cont. equations}$$

Current densities

$$\mathbf{j}_\alpha = -z_\alpha^2 \mu_\alpha \alpha \nabla \varphi_\alpha$$
$$= -z_\alpha q (D_\alpha \nabla \alpha + z_\alpha \mu_\alpha \alpha \nabla \psi)$$

State equations

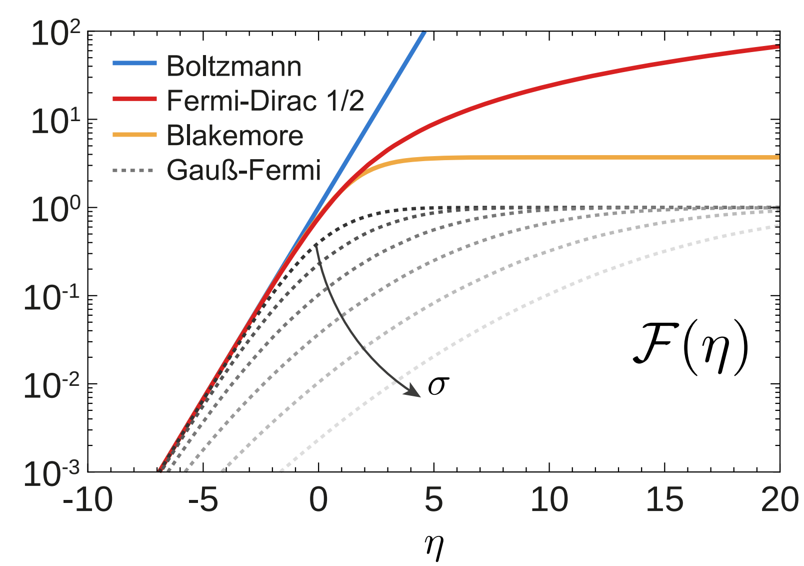
$$\alpha = N_\alpha \mathscr{F}_\alpha(\eta_\alpha), \quad \eta_\alpha = \left(z_\alpha \frac{\psi - \varphi_\alpha - E_\alpha/q}{U_T} \right)$$

Perovskite layer

$$-\nabla \cdot (\varepsilon_s \nabla \psi) = q\,\big(C + p - n + a\big) \qquad \text{Poisson}$$

$$q\partial_t n - \nabla \cdot \mathbf{j}_n = q(G - R),$$
$$q\partial_t p + \nabla \cdot \mathbf{j}_p = q(G - R), \qquad \text{Cont. equations}$$
$$q\partial_t a + \nabla \cdot \mathbf{j}_a = 0$$

Statistics



$$e^\eta$$

$$\frac{1}{e^{-\eta} + 1}$$

$$\frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\xi^{1/2}}{e^{\xi - \eta} + 1}\, \mathrm{d}\xi$$

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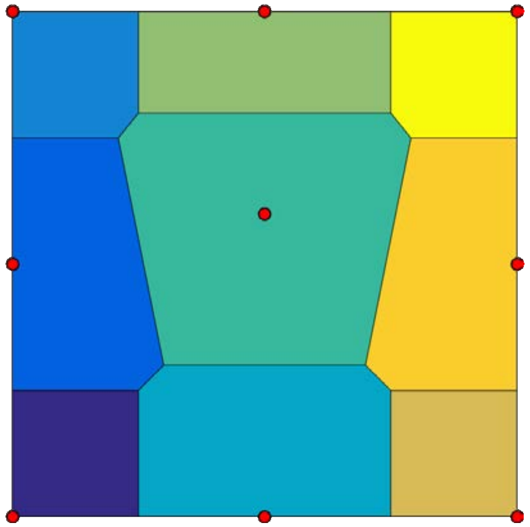
Finite volume discretization

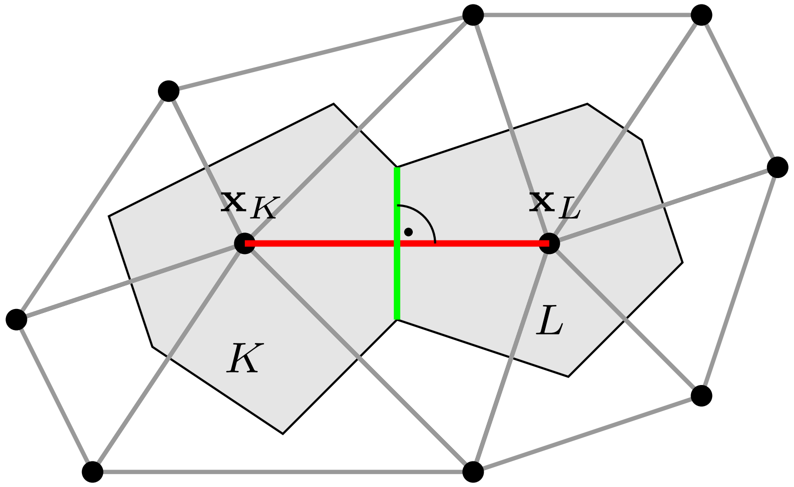
$$\nabla \cdot (\varepsilon \nabla \psi) + q(C + p - n) = 0$$

$$\frac{\partial}{\partial t} n - \frac{1}{q} \nabla \cdot \mathbf{j}_n - (G - R(n,p)) = 0$$

$$\frac{\partial}{\partial t} p + \frac{1}{q} \nabla \cdot \mathbf{j}_p - (G - R(n,p)) = 0$$



Voronoi tessellation



Flux along 1D edge

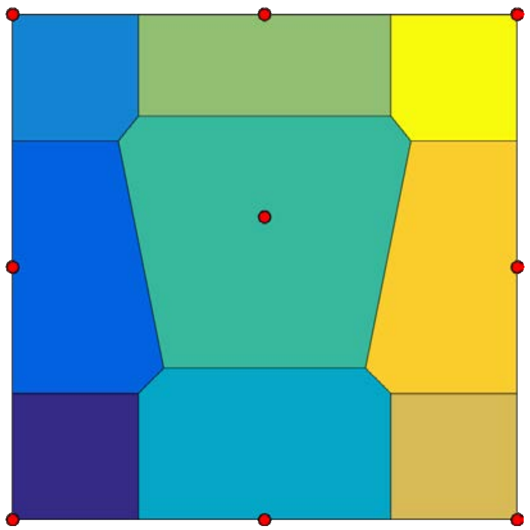
D. Abdel, C. Chainais-Hillairet, P. Farrell, M. Herda. *Numerical analysis of a finite volume scheme for charge transport in perovskite solar cells*. IMA Journal of Numerical Analysis, 2023

Finite volume discretization

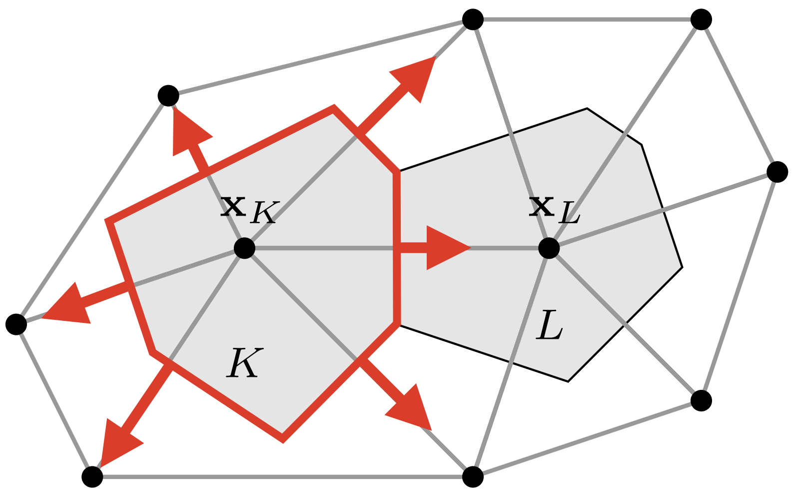
$$\sum_{L\in N(K)} \sigma_{KL}\,(\mathbf{x}_L - \mathbf{x}_K)\cdot(\varepsilon(\psi_L - \psi_K)/h_{K,L}) + q\,|K|\,(C_K + p_K - n_K) = 0$$

$$\frac{\partial}{\partial t}|K|\,n_K - \frac{1}{q}\sum_{L\in N(K)} |\sigma_{KL}|\,j_{n,KL} - |K|\,(G_K - R(n_K, p_K)) = 0$$

$$\frac{\partial}{\partial t}|K|\,p_K + \frac{1}{q}\sum_{L\in N(K)} |\sigma_{KL}|\,j_{p,KL} - |K|\,(G_K - R(n_K, p_K)) = 0$$



Voronoi tessellation



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Existence of solutions

Continuous PDE model

- **Regularized** state equations and reaction terms
- Solvability shown by using discrete arguments and passing to the continuous limit
- **Moser iteration** technique leads to a prior estimates for densities and potentials, independent of the regularisation level
- Existence of the original problem

Discrete FVM model

- SEDAN flux approximation (**Scharfetter-Gummel** type)
- Numerical **entropy-dissipation** relation
- Ensures a priori estimates for the densities and potentials
- Existence of numerical solution via **Brouwer's fixed point theorem**
- Open-source software tool: ChargeTransport.jl

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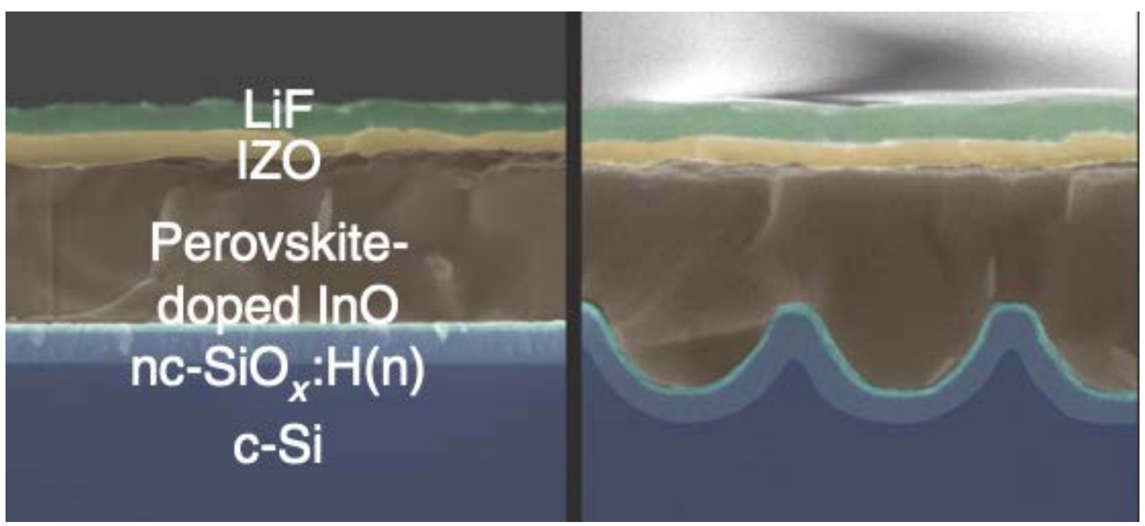
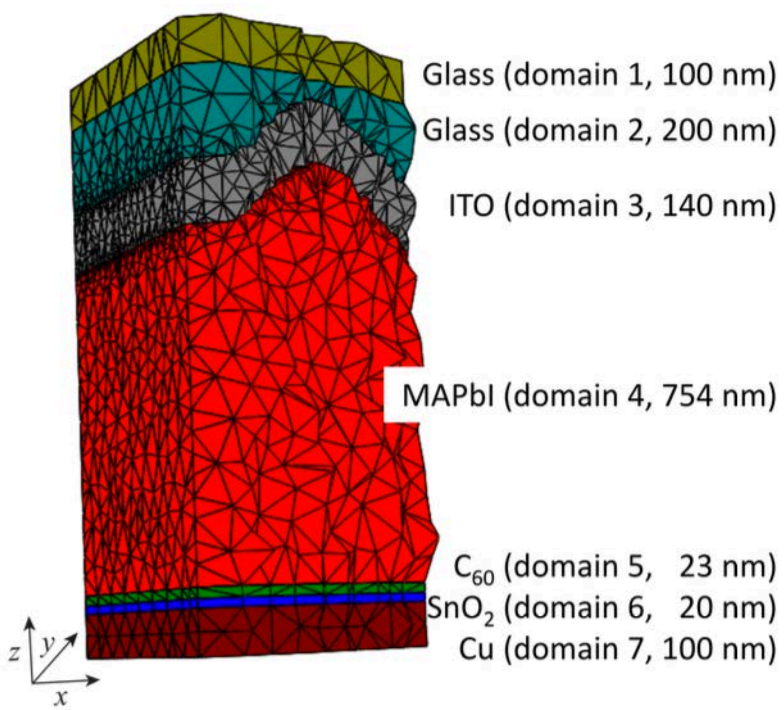
Simulation

- 3D nanotextured perovskite solar cell
- current project with Helmholtz Zentrum and Zuse Institute
- solution converges quadratically in space, linear in time
- relative entropy decays exponentially (as predicted by theory)



planar interface nanotextured



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