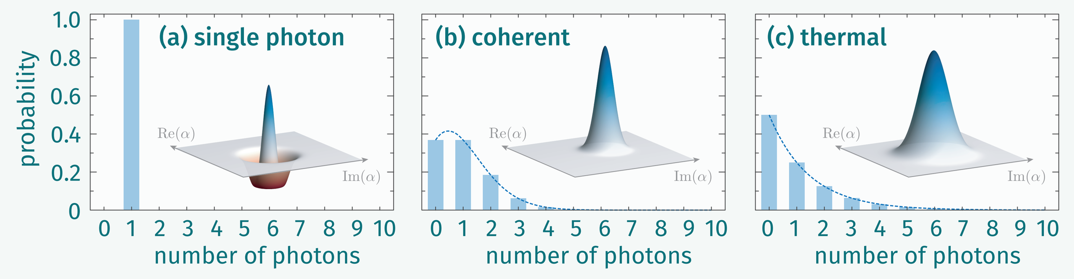
Modeling of Quantum Light Emitting Diodes

Markus Kantner and Uwe Bandelow (WIAS)

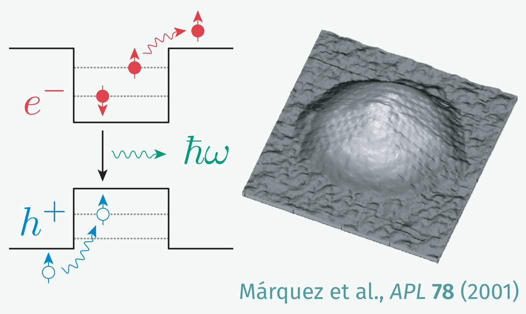
Berlin Mathematics Research Center MATH+

Quantum light for quantum technologies

- motivation:
  - photons as optical **qubits** (units of quantum information) for quantum information processing and **quantum computing**
  - secure communication based on **quantum cryptography** using **single photons** or **entangled** photon pairs
  - squeezed light for quantum metrology applications
- quantum electrodynamics: particle-like properties (discrete excitations) of electromagnetic field beyond Maxwell theory



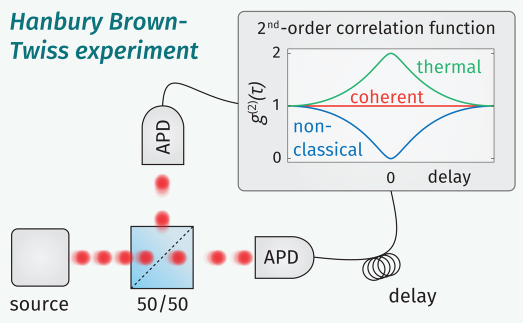
- semiconductor **quantum dots**
  - 3D confinement of wave functions: **"artificial atoms"**
  - integration in photonic microcavities: **Purcell effect**



Márquez et al., APL 78 (2001)

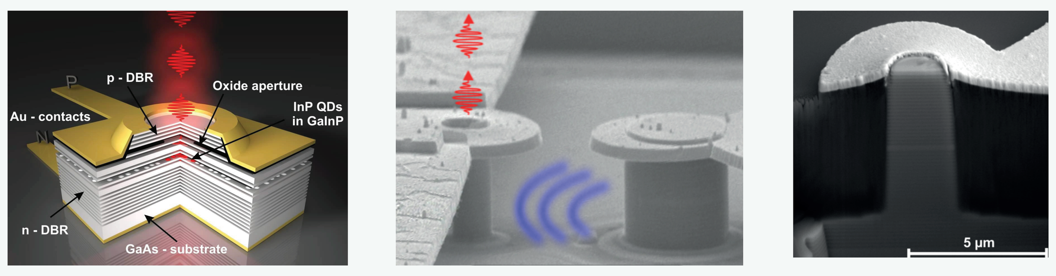
- coherence of the optical field
  - 2[nd]-order intensity auto-correlation function $g^{(2)}(\tau)$
  - **photon-antibunching:** sub-Poissonian variance, non-classical state of light

$$g^{(2)}(\tau)=\frac{\langle a^{\dagger}(0)\,a^{\dagger}(\tau)\,a(\tau)\,a(0)\rangle}{\langle a^{\dagger}(0)\,a(0)\rangle^{2}}$$



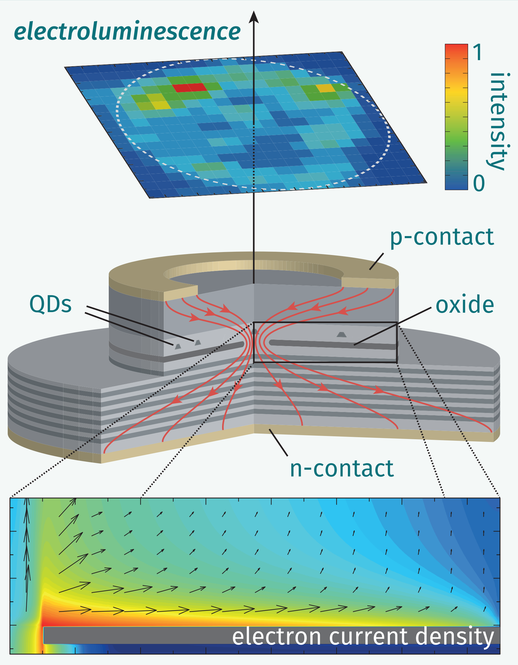
- **electrically driven devices** for real-world applications
  - quantum dots in diodes
  - excitation via on-chip integrated (few QD) nanolasers

Florian, PhD thesis, University of Bremen (2014)
Munelly et al., ACS Photonics 4, 790–794 (2017)
Reitzenstein & Forchel, J. Phys. D 43, 033001 (2010)



Current injection in oxide-confined QD-diodes

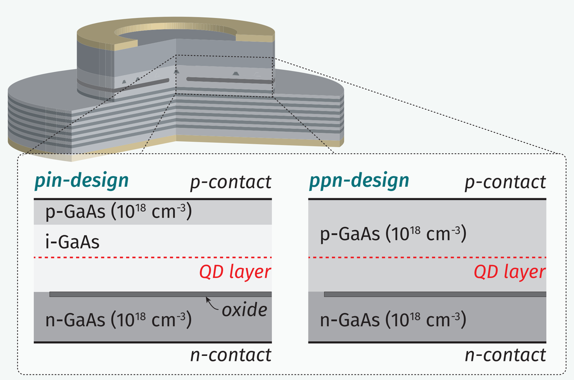
- device concept:
  - buried stressor (oxide) for site-controlled QD nucleation and current funneling to central QD
  - lower DBR-mirror section for directional emission
- problem: optical activity of several parasitic QDs
- simulation of current flow using **drift-diffusion system**

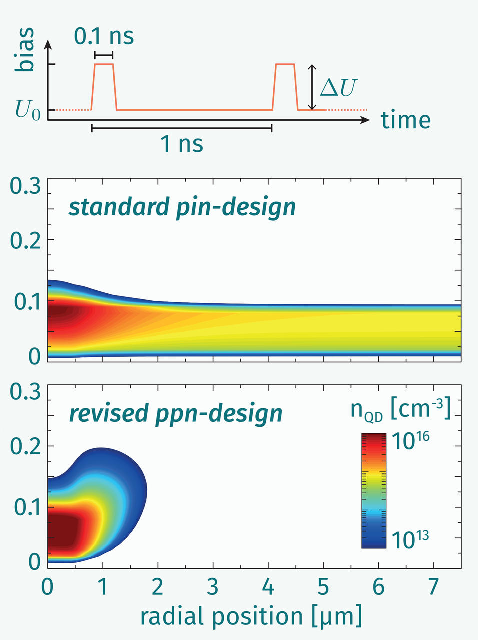


$$-\nabla\cdot\varepsilon\nabla\phi=q\,(C+p-n)$$
$$\partial_t n-\frac{1}{q}\nabla\cdot\mathbf{j}_n=-R$$
$$\partial_t p+\frac{1}{q}\nabla\cdot\mathbf{j}_p=-R$$

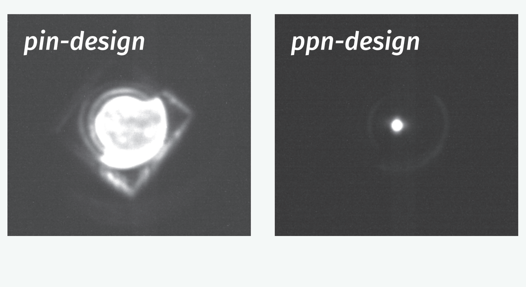
numerical simulation reveals lateral **current spreading** [10]
+ low injection regime
+ cryogenic temperature

- **doping modification** [10]
  - p-doping of active region ("ppn-design")
  - → reduced lateral current spreading due to increased carrier recombination rate



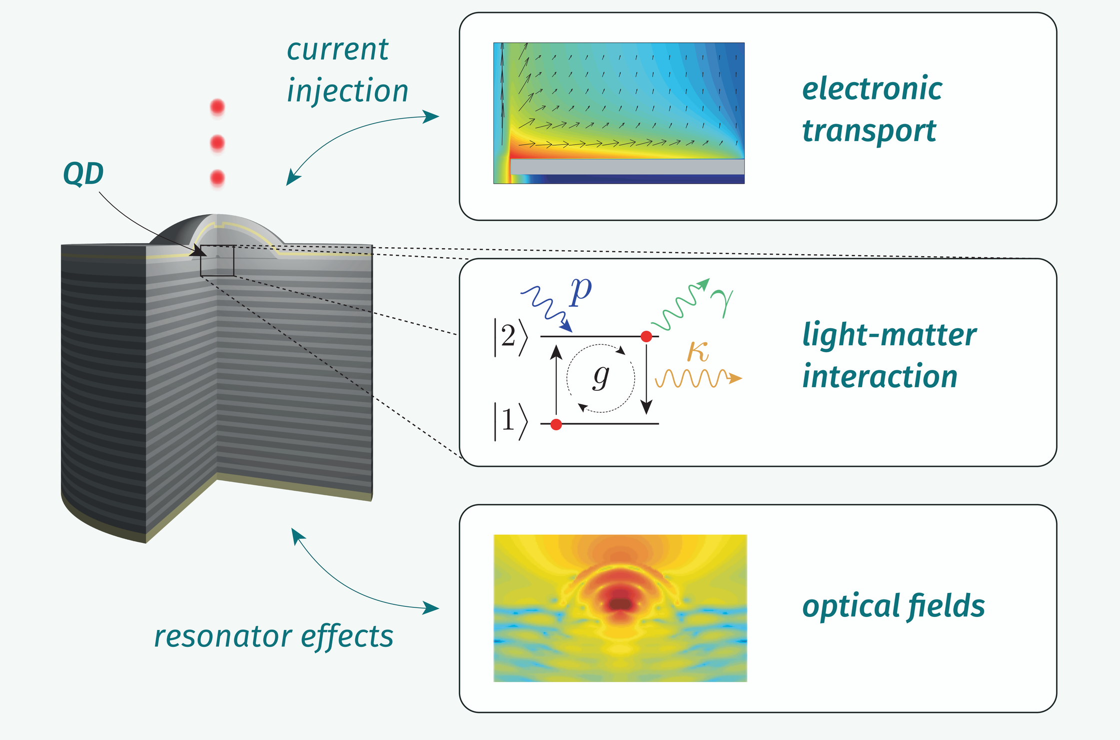


- **experimental verification** [2]
  - revised design (ppn) with superior confinement of injection current
  - **electrical control of single quantum dots!**



conclusions:
+ semi-classical carrier transport simulation useful for optimization of quantum light souces
- no description of quantum optical properties

Multi-physics device-scale simulation

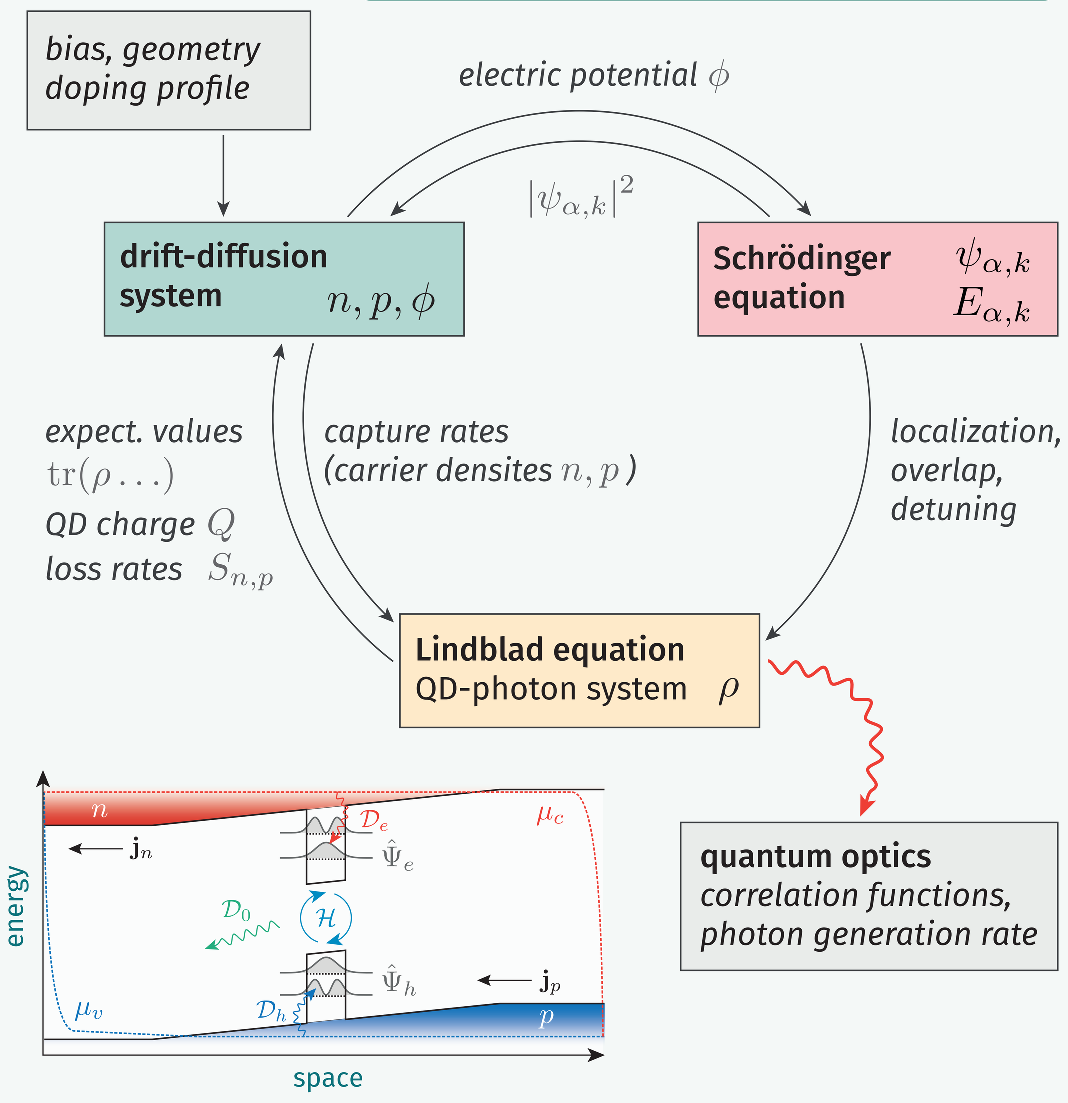


Quantum-classical modeling approach

Schrödinger-Poisson-Drift-Diffusion-Lindblad system [3, 5, 6, 7]

Semi-classical carrier transport + cavity-quantum electrodynamics out of one box!

$$-\nabla\cdot\varepsilon\nabla\phi=q\,(C+p-n)+Q$$
$$\partial_t n-\frac{1}{q}\nabla\cdot\mathbf{j}_n=-R-S_n$$
$$\partial_t p+\frac{1}{q}\nabla\cdot\mathbf{j}_p=-R-S_p$$
$$\mathcal{H}_\alpha\psi_{\alpha,i}=E_\alpha\psi_{\alpha,i}\qquad(\alpha\in\{e,h\})$$
$$\partial_t\rho=-\frac{i}{\hbar}[H,\rho]+\mathcal{D}(\rho)$$



- **Lindblad master equation**
  - fully quantum mechanical light-matter interaction beyond semi-classical approximation (Jaynes–Cummings model)
  - Coulomb interaction between QD-bound carriers
  - dissipative interactions with macroscopic carrier reservoir (carrier capture/ escape, spont. emission, dephasing)
  - out-coupling of cavity photons
- (stationary) **Schrödinger equation**
  - eigenfunctions and -values depending on state of macroscopic environment (device's internal electric field)
  - quantum confined Stark effect
  - adiabatically adapting state space for density matrix
- **feedback on macroscopic system**
  - charge density Q of quantum system modifies electrostatic environment (Coulomb interaction)
  - loss rates $S_{n/p}$ balance carriers scattered to QD states

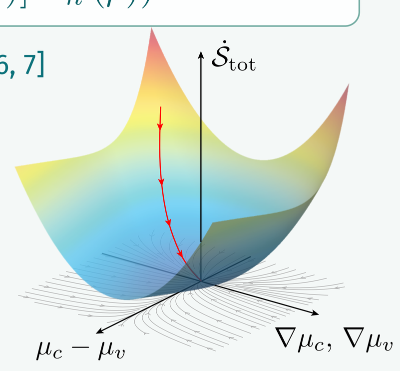
Consistency with thermodynamics

- dissipation rate of fully coupled quantum-classical system

$$0\le\dot{\mathcal{S}}_{\mathrm{tot}}=\frac{1}{T}\int_\Omega\mathrm{d}V\,\left([\mu_c-\mu_v]\,R+\frac{1}{q}\mathbf{j}_n\cdot\nabla\mu_c+\frac{1}{q}\mathbf{j}_p\cdot\nabla\mu_v\right)$$
$$+k_B\,\mathrm{tr}\left([\log\rho-\beta H]\,\mathcal{D}_0(\rho)\right)$$
$$+k_B\,\mathrm{tr}\left([\log\rho-\log\rho_e^*(n,p,\phi)]\,\mathcal{D}_e(\rho)\right)$$
$$+k_B\,\mathrm{tr}\left([\log\rho-\log\rho_h^*(n,p,\phi)]\,\mathcal{D}_h(\rho)\right)$$

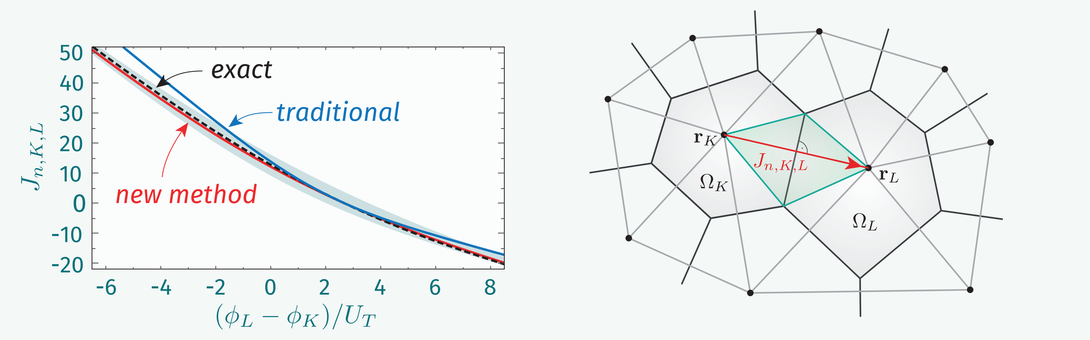
→ **obeys 2[nd] law of thermodynamics!** [6, 7]

- thermodynamic equilibrium: minimization of **hybrid grand potential** (classical + quantum functional)
- quantum detailed balance relation
- consistency with **GENERIC** [4, 6]

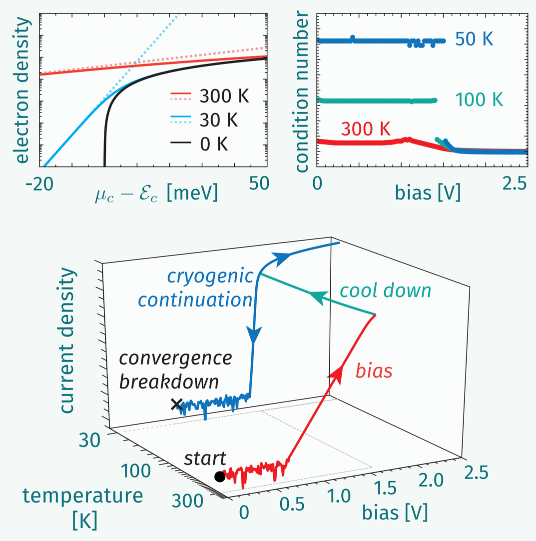


Numerical methods

- Voronoï box-based **finite volume method** [6, 8]
  - discretization method for balance equations
  - robust + accurate **Scharfetter–Gummel scheme** for strongly degenerate semiconductors **(Fermi–Dirac statistics)** [1, 3, 6]



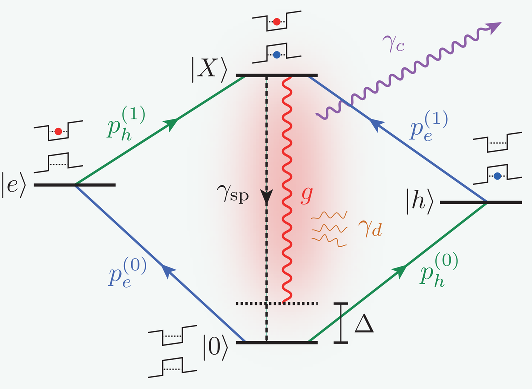
- **cryogenic temperature** [3, 9]
  - carrier density freeze-out: numerical underflow → *ill-conditioned system*
  - **temperature-embedding method**: circumvent intractable parameter regime
- **non-local** quantum-classical **coupling**: Jacobian sparsity [6]

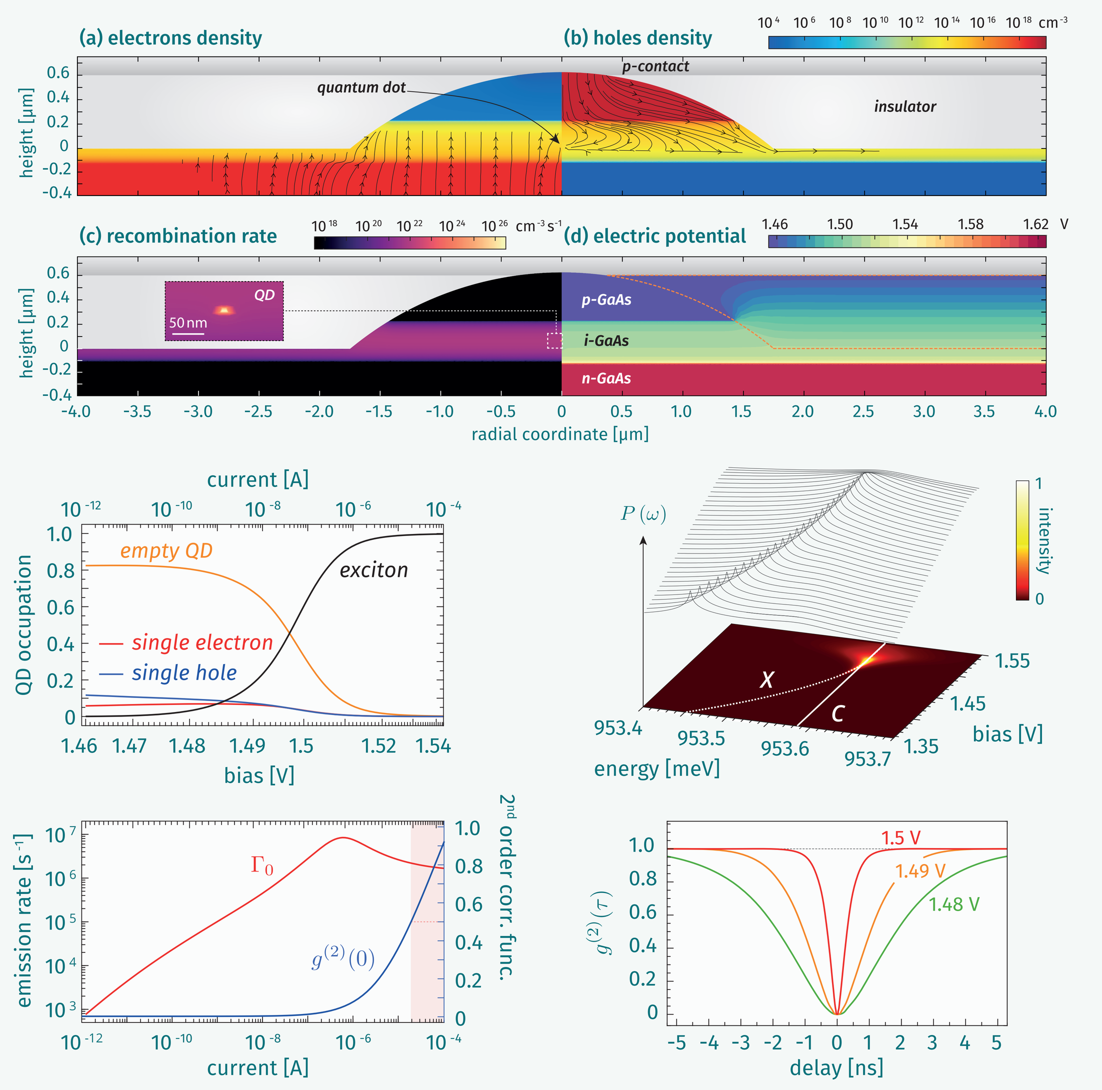


Simulation results

Demonstration of quantum-classical modeling approach by numerical simulation of single-photon emitting diode [3, 5]

- Hamiltonian
  - four electronic QD states
  - single cavity mode
  - Coulomb interaction
  - Jaynes–Cummings-type exciton-photon coupling
- dissipation superoperator
  - carrier capture
  - cavity-photon emission
  - pure dephasing





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contact: Markus Kantner · Weierstrass Institute for Applied Analysis and Stochastics · Mohrenstraße 39, D-10117 Berlin, Germany · kantner@wias-berlin.de · phone: +49 (30) 20372-504 · fax: +49 (30) 20372-318 · https://www.wias-berlin.de/people/kantner