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Si:P δ-layer Resonant Tunnel Junctions for TeraHertz applications

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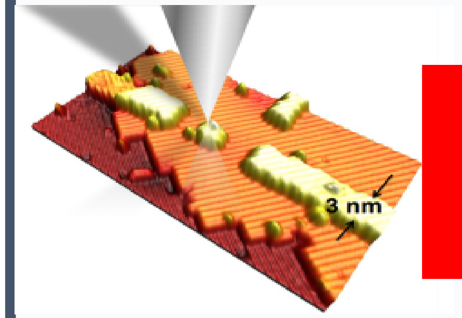
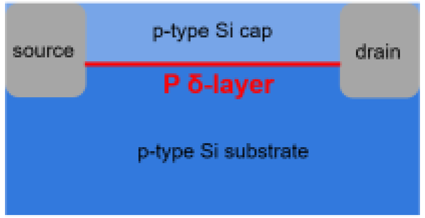
Atomic Precision Advanced Manufacturing (APAM)

APAM

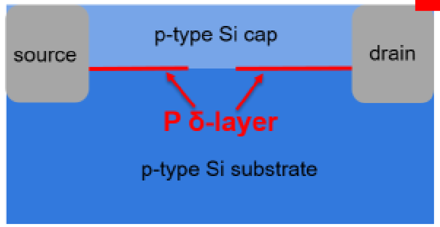


STM = Scanning Tunneling Microscope

APAM devices



Si: P δ-layer wire



Si: P δ-layer Tunnel Junction

APAM Applications

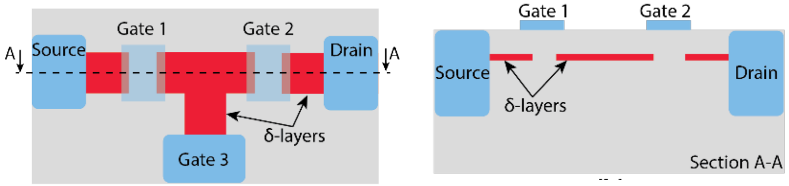
- **Beyond Moore Computing**

NANO LETTERS

pubs.acs.org/NanoLett Letter

Monolithic Three-Dimensional Tuning of an Atomically Defined Silicon Tunnel Junction

Matthew B. Donnelly,* Joris G. Keizer, Yousun Chung, and Michelle Y. Simmons



δ-layer tunnel junction FET

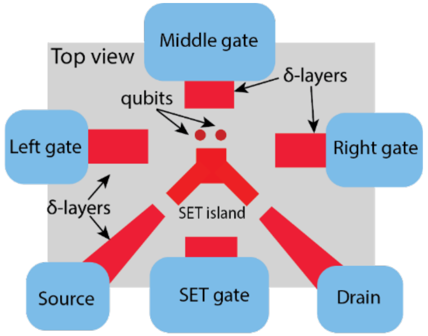
- **Quantum Computing**

LETTER

https://doi.org/10.1038/s41586-019-1381-2

A two-qubit gate between phosphorus donor electrons in silicon

Y. He[1,2], S. K. Gorman[1,2], D. Keith[1], L. Kranz[1], J. G. Keizer[1] & M. Y. Simmons[1]*



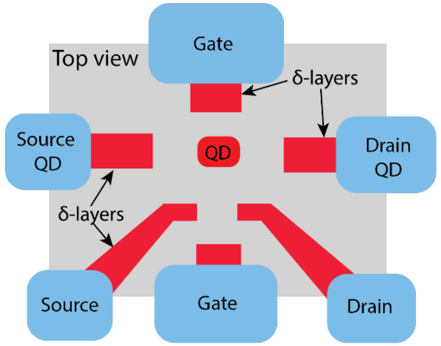
- **Novel quantum sensing**

APPLIED PHYSICS LETTERS **104**, 113111 (2014)

Single-charge detection by an atomic precision tunnel junction

M. G. House,[a)] E. Peretz, J. G. Keizer, S. J. Hile, and M. Y. Simmons[b)]

Centre for Quantum Computation and Communication Technology, University of New South Wales, Sydney, NSW 2052, Australia



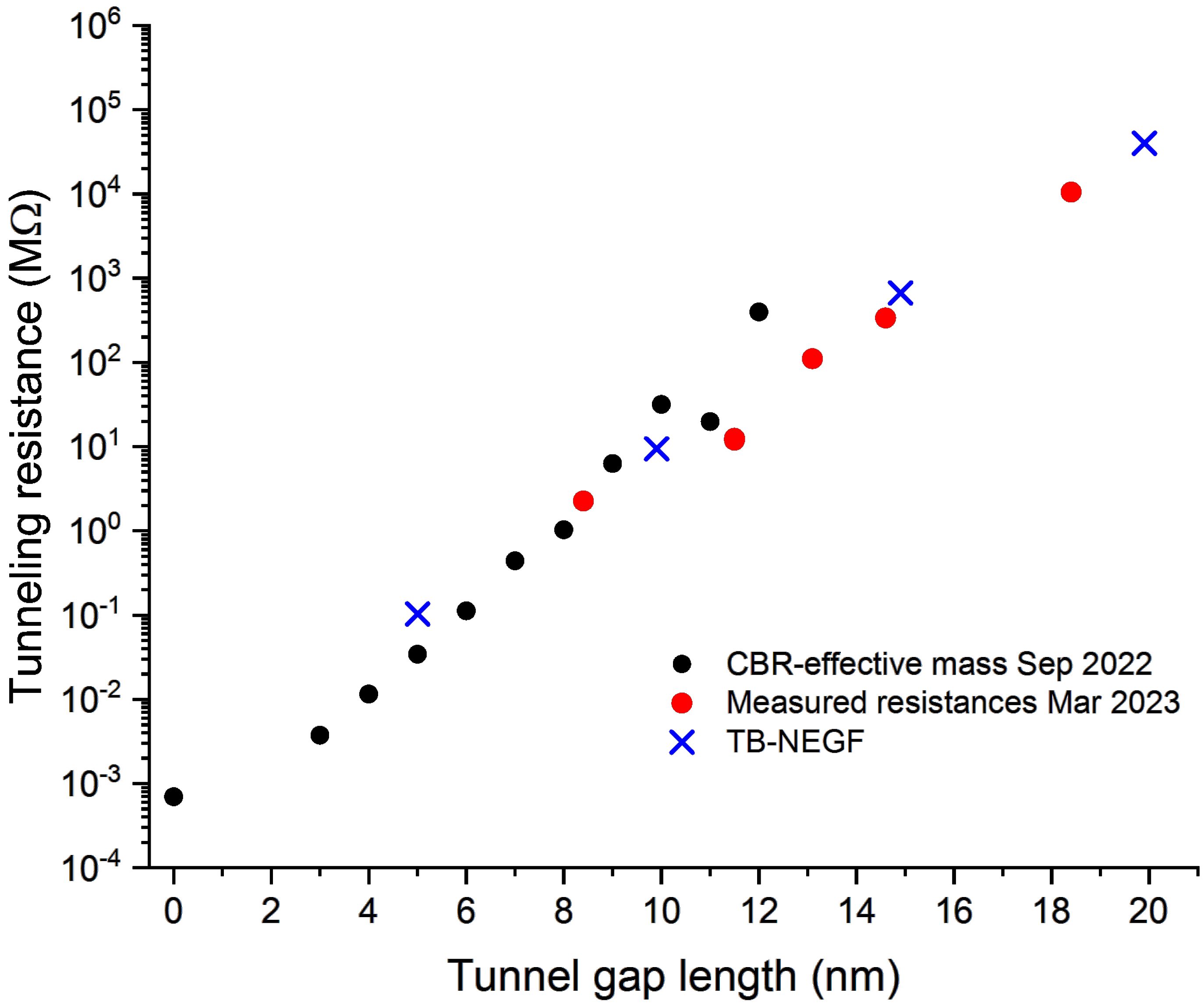
Computational approach, validation, predictive transport simulation for Si:P delta-layer systems

- Charge self-consistent NEGF implemented via Contact Block Reduction method scales linearly with the simulation volume O(V)
- Electron-electron interaction via DFT-LDA exchange-correlation
- Kinetic energy term: the effective mass tensor
- Real-space scattering on discrete impurities

This approach allows to accurately represent all *open-system electron properties* of highly-conducting highly-confined systems*:*

1. D. Mamaluy, J. P. Mendez *et al. Commun Phys* 4, 205 (2021)
2. J. P. Mendez, D. Mamaluy, *Sci Rep* 12, 16397 (2022)
3. J. P. Mendez, S. Misra, and D. Mamaluy, Phys. Rev. Applied 20, 054021 (2023).

Predictive quantum transport simulations



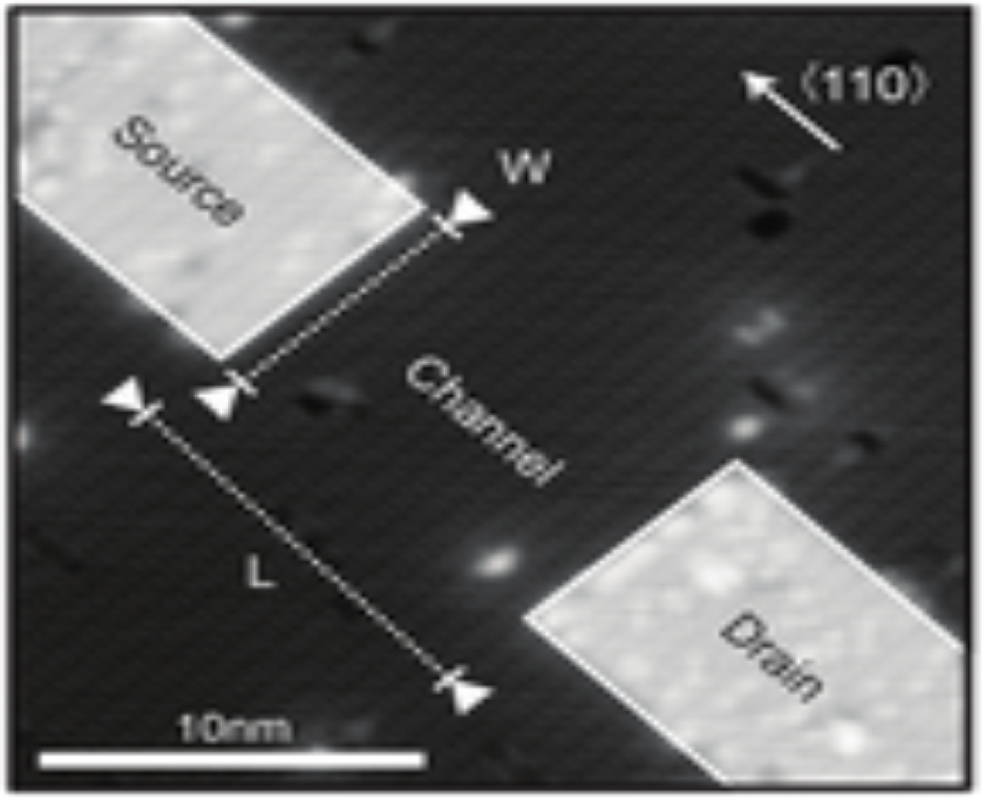
ADVANCED FUNCTIONAL MATERIALS

Research Article | Open Access

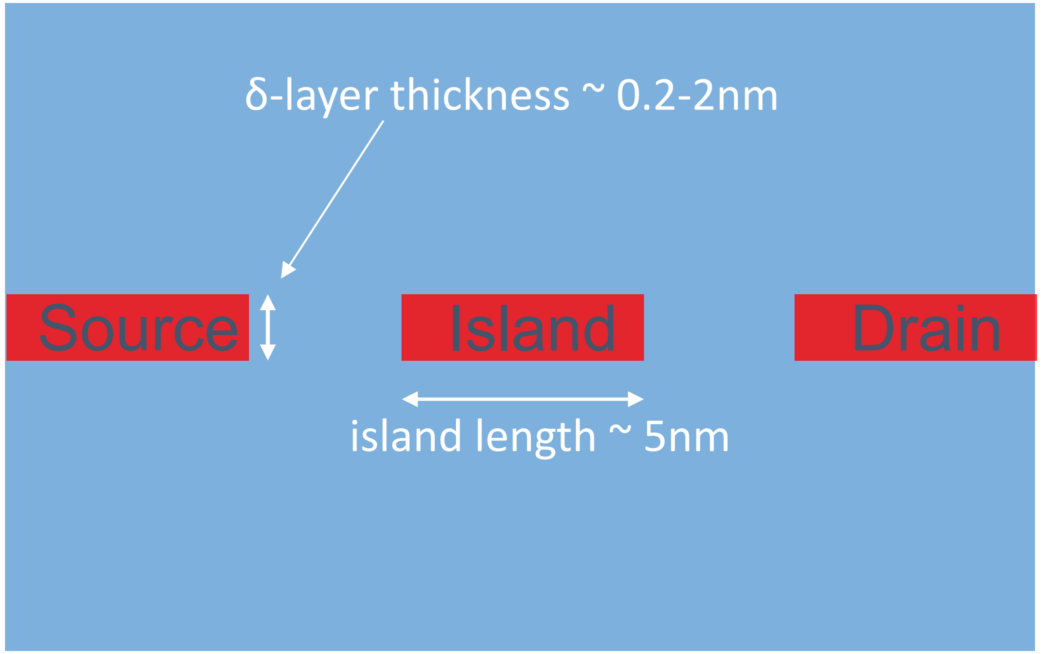
Multi-Scale Modeling of Tunneling in Nanoscale Atomically Precise Si:P Tunnel Junctions

Matthew B. Donnelly, Mushita M. Munia, Joris G. Keizer, Yousun Chung, A. M. Saffat-Ee Huq, Edyta N. Osika, Yu-Ling Hsueh, Rajib Rahman, Michelle Y. Simmons

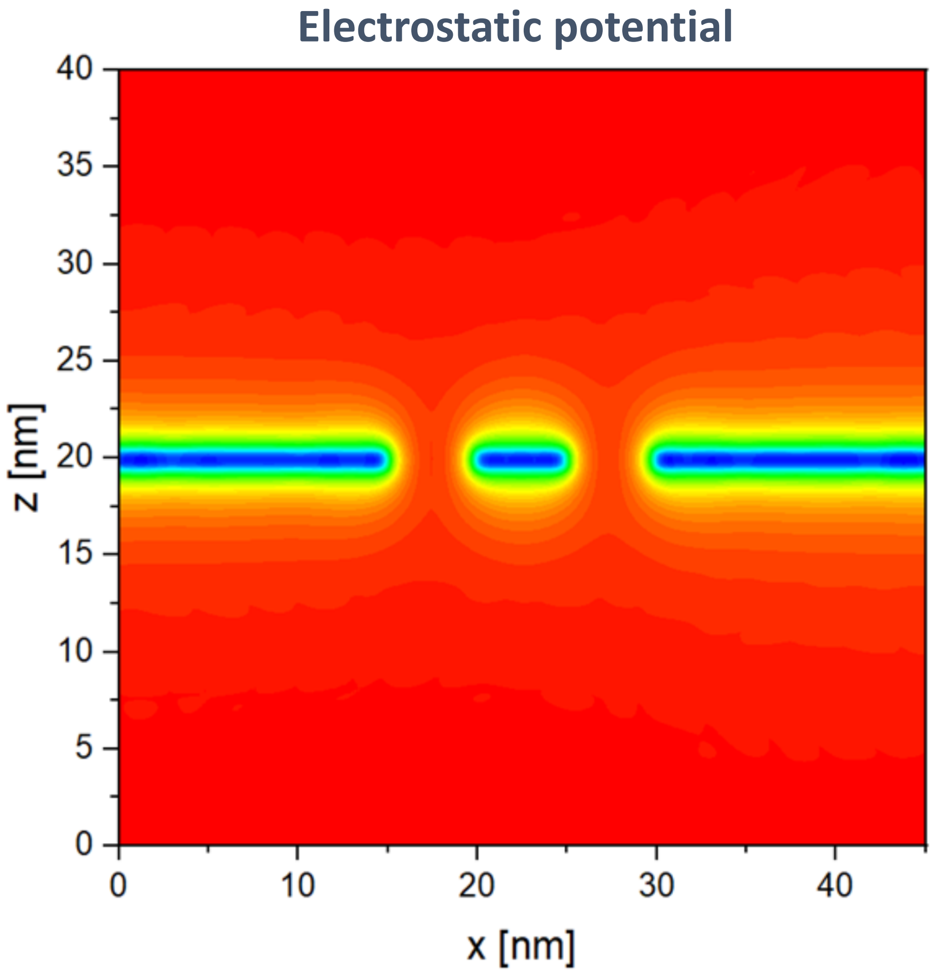
First published: 08 March 2023 | https://doi.org/10.1002/adfm.202214011



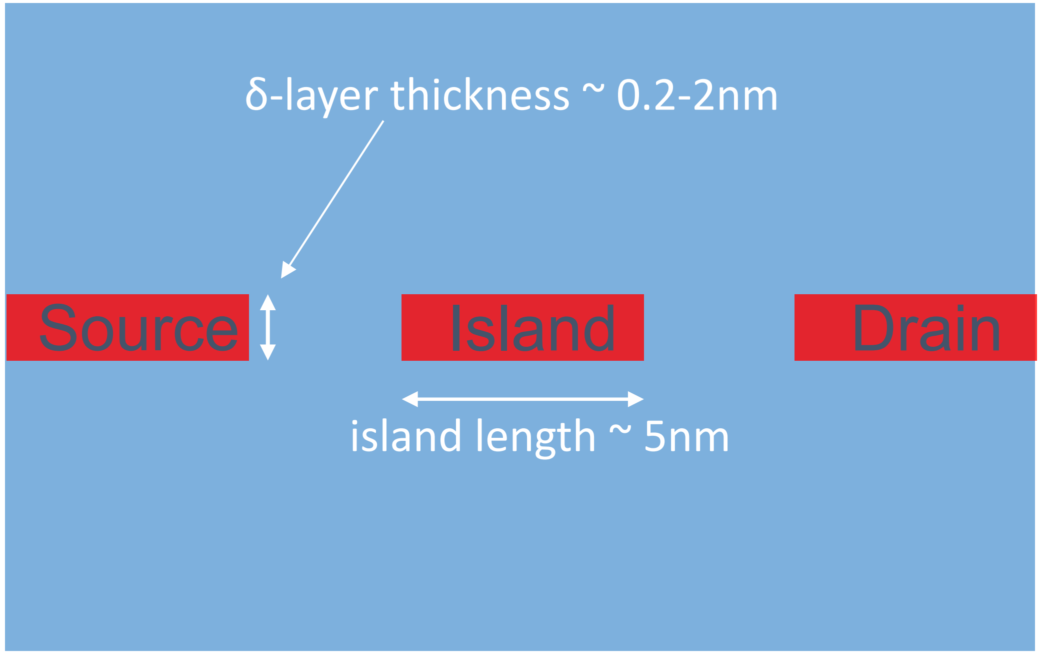
δ-layer Resonant Tunneling Junction devices

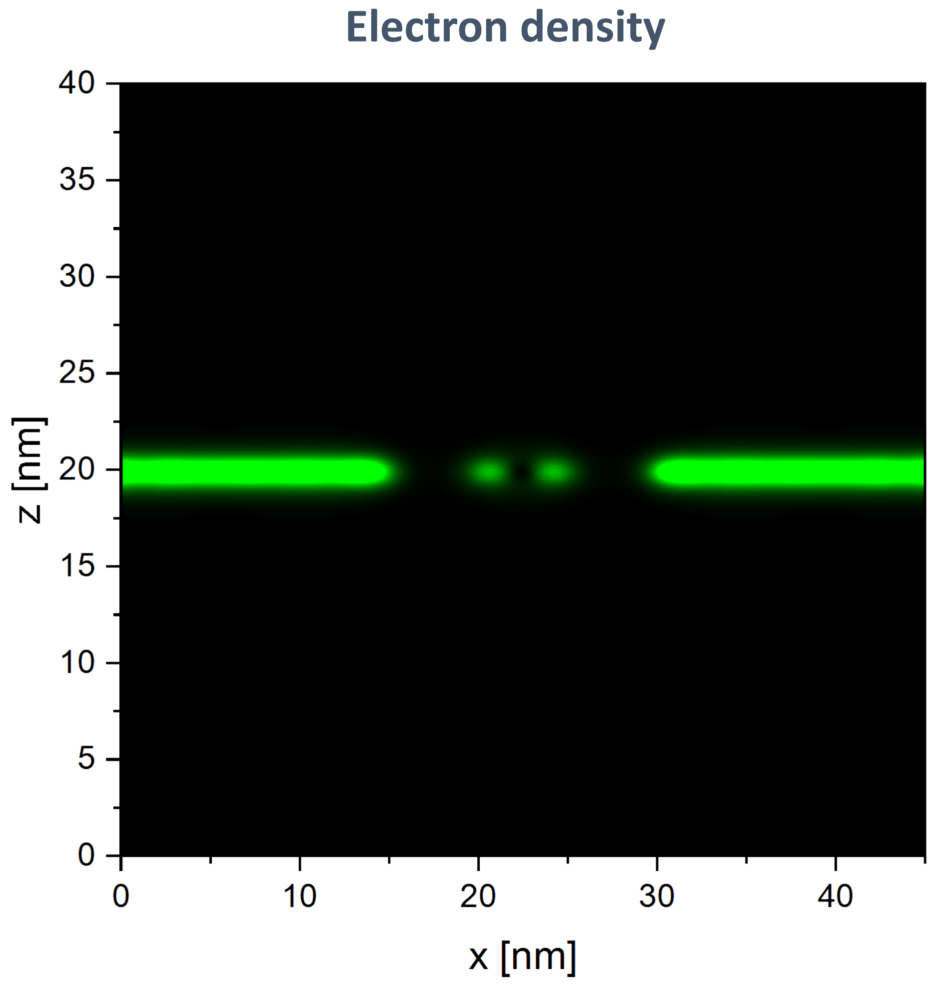


Two-terminal device: $J=J(V_{DS})$



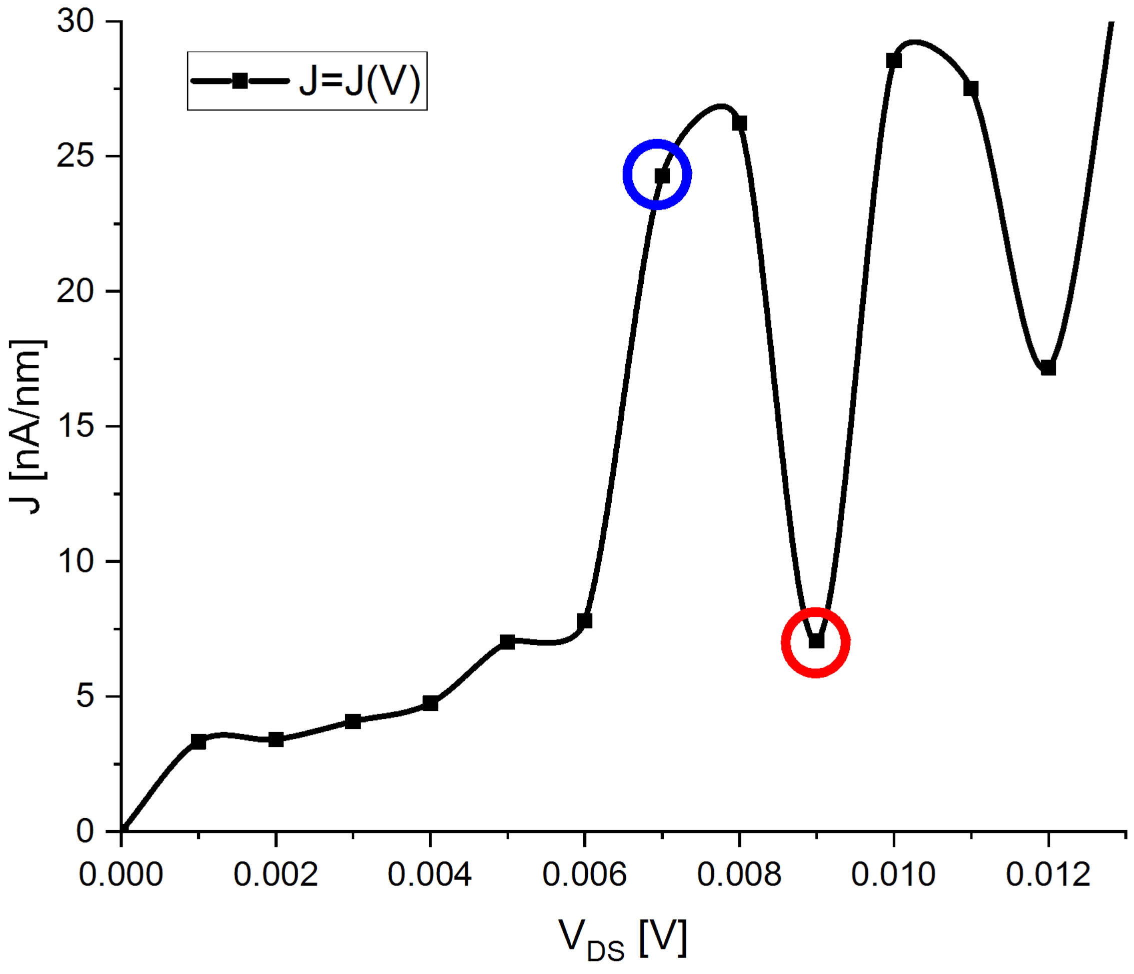
δ-layer Resonant Tunneling Junction devices

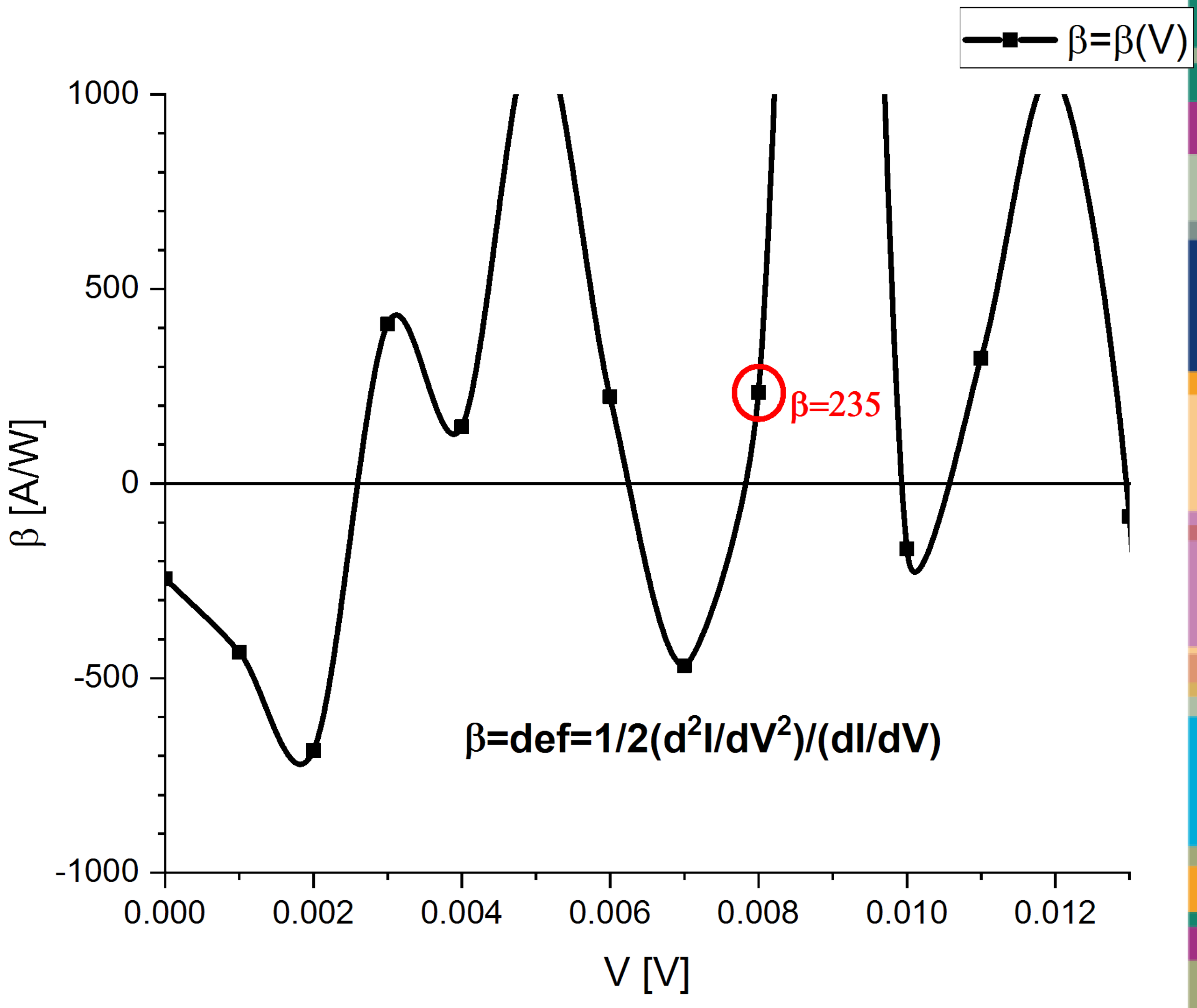




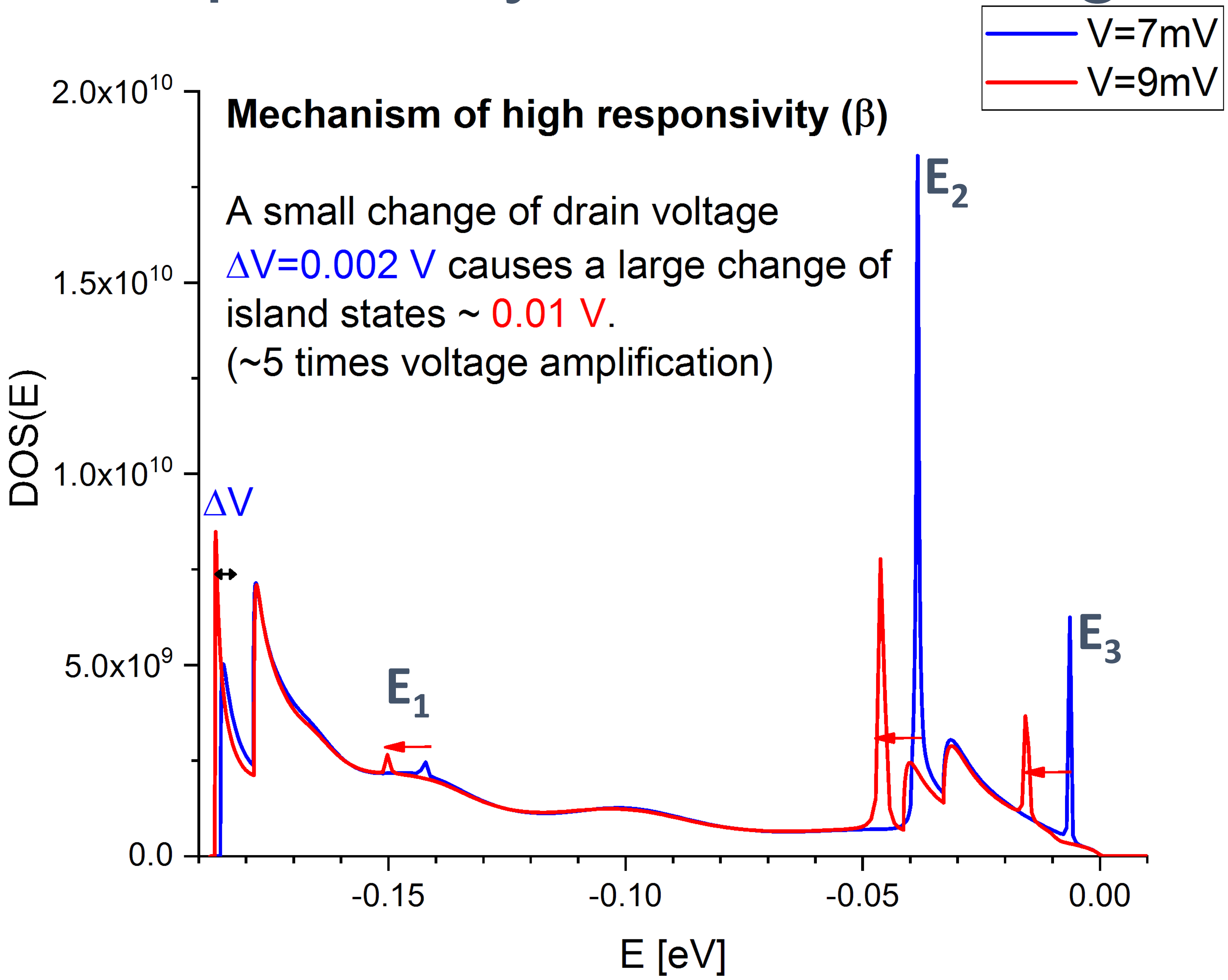
Two-terminal device: $J=J(V_{DS})$

Electrical characteristics: strong NDR, extremely high responsivity (β)

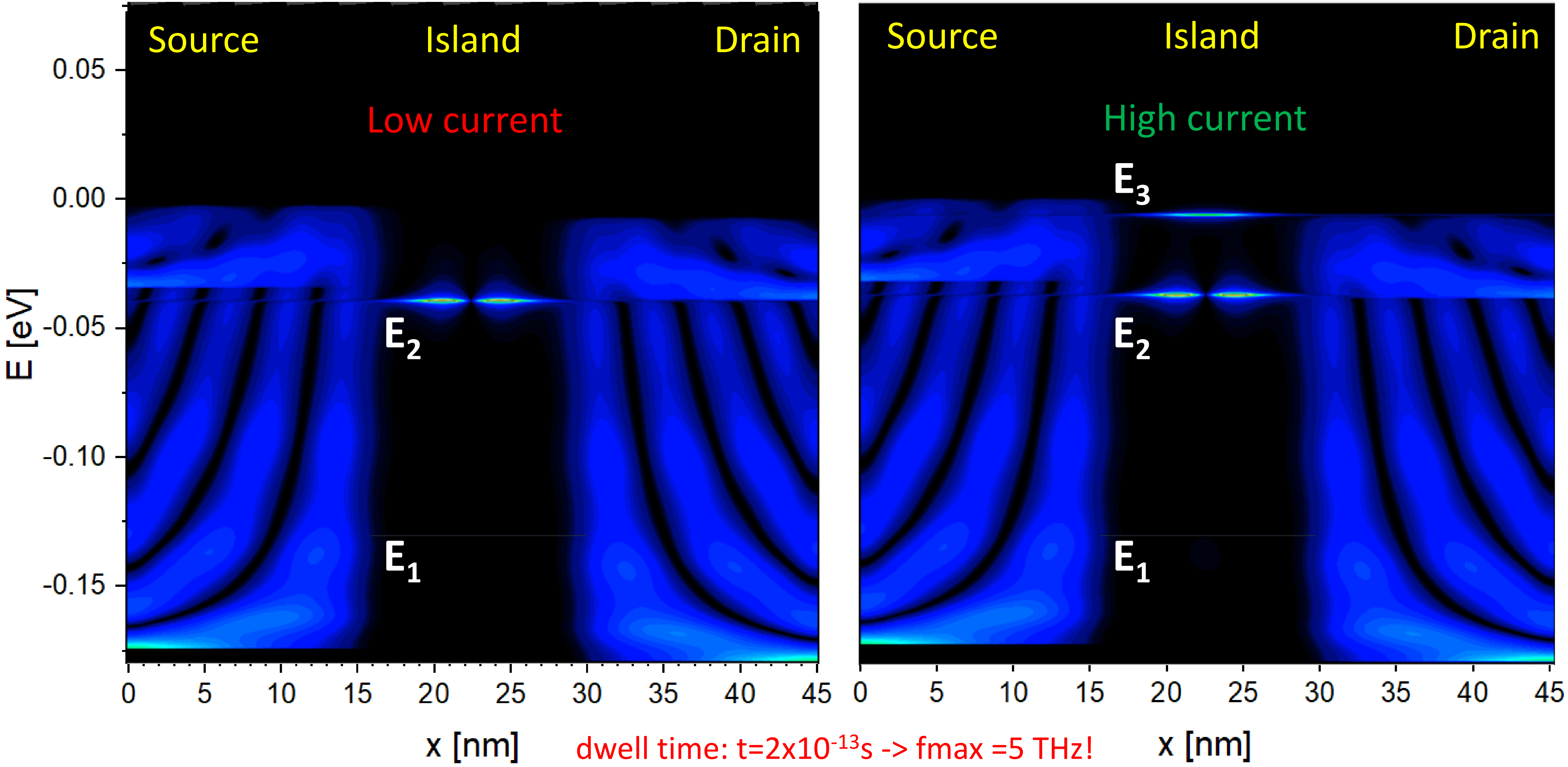




High responsivity and the change in DOS

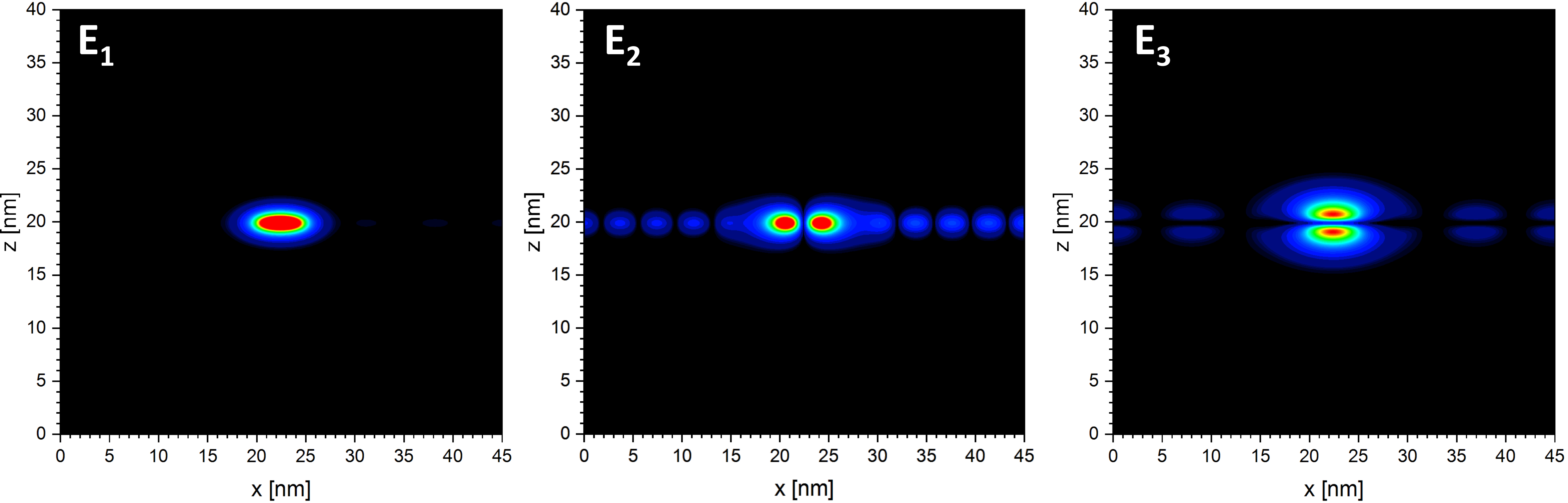


LDOS: “Off” and “on” states



dwell time: $t = 2 \times 10^{-13}$ s -> fmax =5 THz!

Quasi-bound and resonant states



Efficient convergence of the charge self-consistent loop requires a special treatment of quasi-bound and resonant states.

Conclusions

- 1) We have created a truly *predictive*, open-system quantum transport simulator for silicon-based devices.
- 2) Negative differential resistance devices (NDR) are needed for high efficiency dc-to-ac current conversion.
- 3) We have proposed a new APAM-based NDR device with TeraHertz operating frequency, good PVR and extremely high responsivity.
- 4) Predictive simulation of NDR devices benefits from a special treatment of quasi-bound and resonant states.