

Metrology Studies with NEMO, a Multimillion Atom Simulation Tool

G. Klimeck¹, J. E. Fonseca¹, R. Rahman¹, N. Kharche², G. P. Lansbergen³, S. Rogge^{3,4}

¹ Network for Computational Nanotechnology, Purdue University, West Lafayette, Indiana, USA

² Brookhaven National Lab, Upton, NY, USA

³ Kavli Institute of Nanoscience, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands

⁴ CQC2T, University of New South Wales, Sydney, NSW 2052, Australia

If you need modeling & simulation insights, ask for NEMO

getnemo5@gmail.com

From Atoms to Devices: NEMO5

Free, multiscale, multipurpose, highly parallel semiconductor nanodevice simulation tool

NEMO5 - Multi scaling transport capability
Tunable accuracy of NEGF solutions
5 * 5 nm² Si nanowire: up to 1000x faster solution
Novel approach in NEGF (nonequilibrium Green's functions) low rank approximation
Accurate + efficient quantum transport calculations

NEMO - Quantum computing
Single impurities and many particle physics
Potential landscape of a single P in Si
M. Fuechsle et al. Nature nanotechnology 7, 242 (2012)

NEMO5 - Phonons
Near and long range interactions (Keating valence force field + Coulomb)
NEMO5: GaAs bulk phonon dispersion

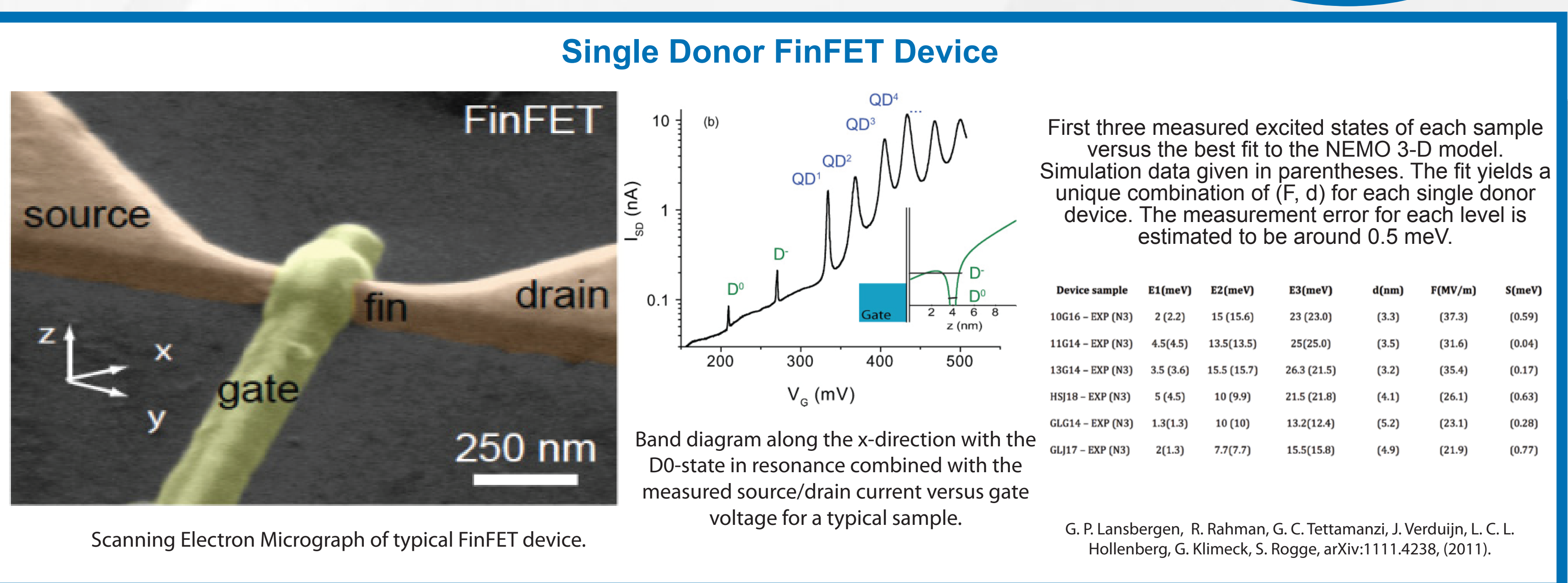
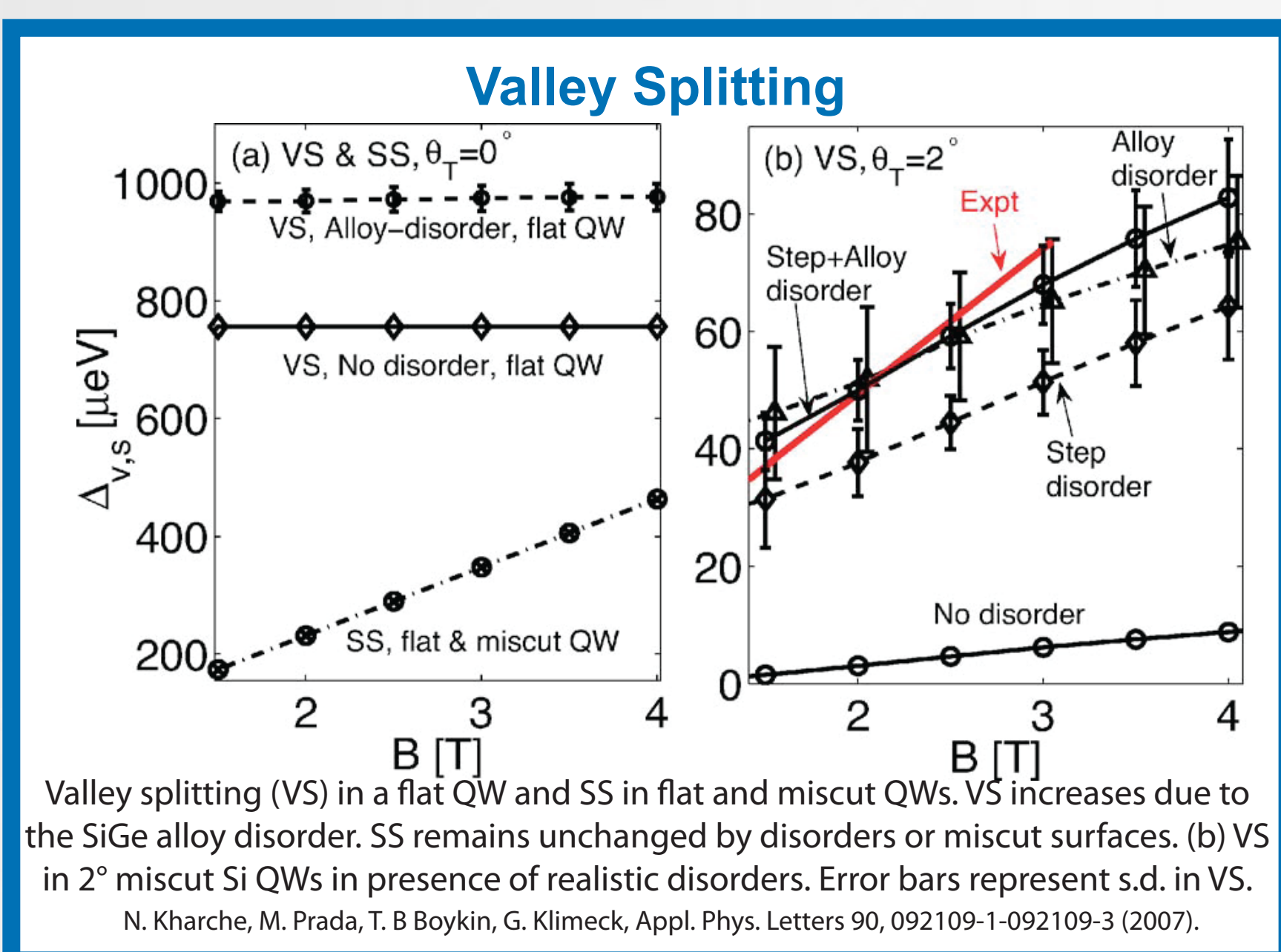
NEMO5 - Electrons in metals
2nd nearest neighbor tight binding Cu, Au, Ag, Al, Pb, etc.
NEMO5: transmission in Cu nanowire

NEMO5 - Spin transport
Topological insulators
Energy (eV) vs k_{||} (1/nm)
*Yi Zang et al. Nature Phys. 6, 584

NEMO5 - Structure Relaxation
~50 Million atoms
InAs dome shaped dot in GaAs

NEMO5 - Device reliability
Random - impurities - alloys - interfaces etc.
Transistor nanowire with rough surface

20% matrix rank 125 x faster
50% matrix rank 90% ... 8 x faster
Heat transport
Spin transport

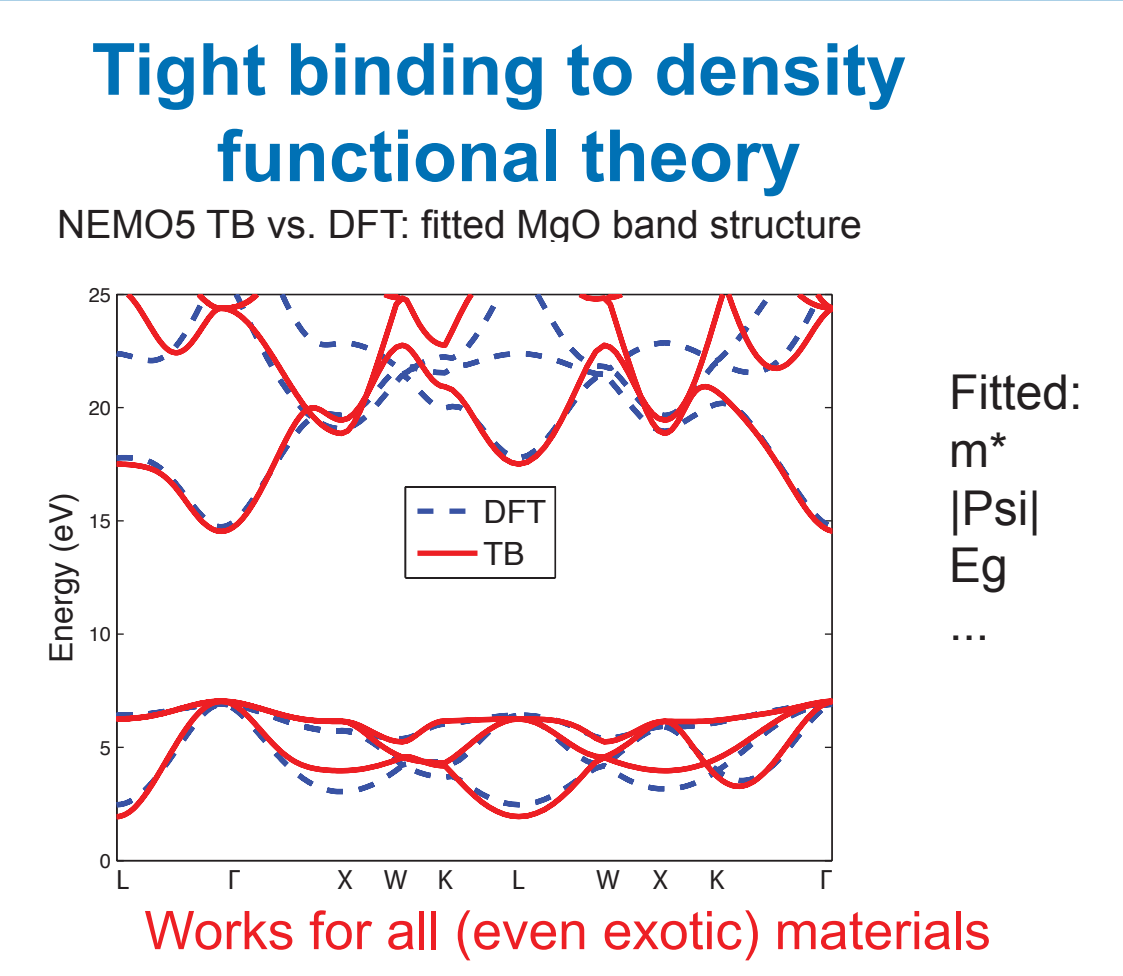
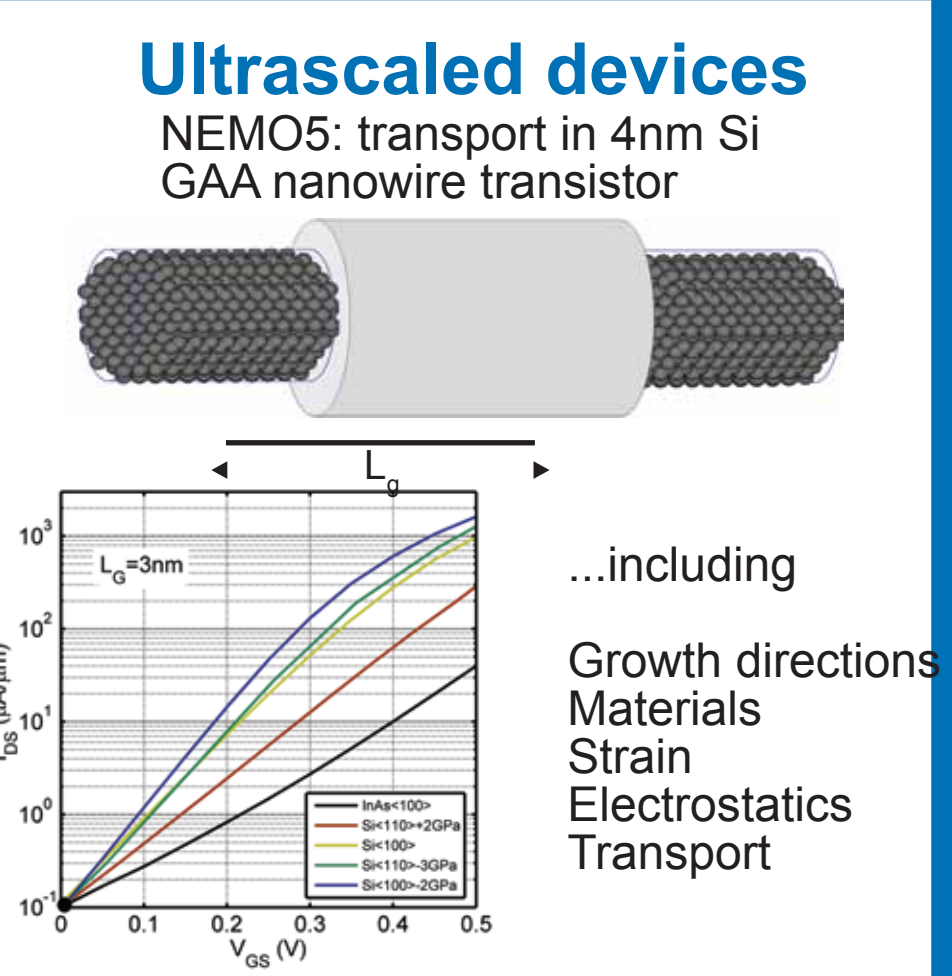
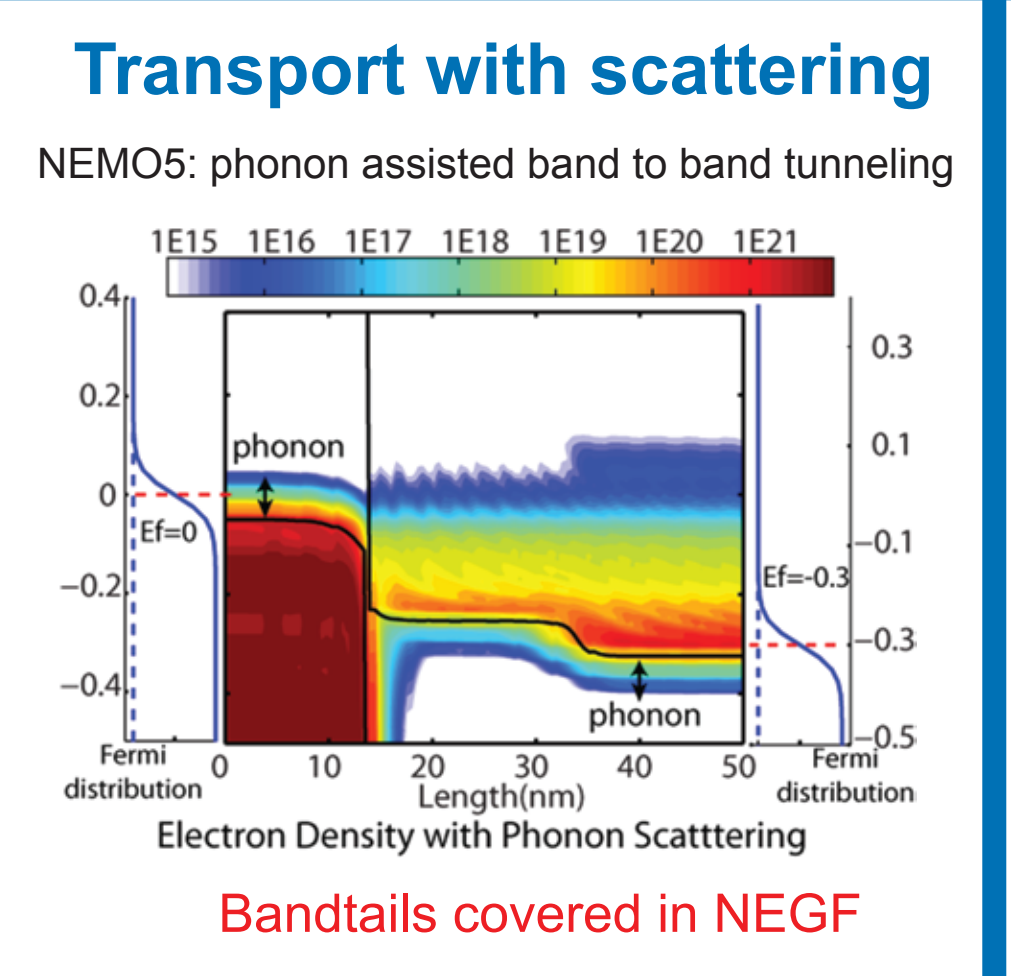


Arbitrary device geometries

0D, 1D, 2D, 3D available (4D in preparation)
NEMO5: samples of device geometries

B. Radisavljevic et al. Nature Nanotechnology 6, 147 (2011)
J. Bai et al. Nature Nanotechnology 5, 190 (2010)

Ready for future device generations



Collaborators

NanoHUB world... 230,000+ users
NEMO based tools: 10,000+ users

Intel, Samsung, GlobalFoundries, IBM, Lockheed Martin, ...