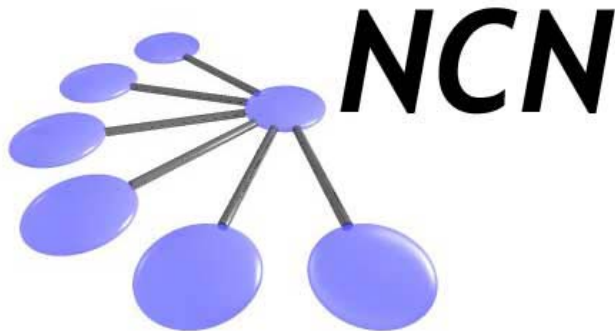


Network for Computational Nanotechnology (NCN)

Berkeley, Univ. of Illinois, Norfolk State, Northwestern, Purdue, UTEP

NEMO1D: Motivation / History / Key Insights



Gerhard Klimeck

Thanks to:
NEMO Core Team Members

NEMO 1-D – 1994-1998

Roger Lake, Texas Instruments / UC Riverside

R. Chris Bowen, Texas Instruments / JPL / TI

Tim Boykin, U Alabama in Huntsville

Dan Blanks, Texas Instruments

William R. Frensley, UT Dallas

NEMO 1-D – 1998-2003

R. Chris Bowen, JPL

Tim Boykin, U Alabama in Huntsville

Post Docs / Students / Developers / Consultants:

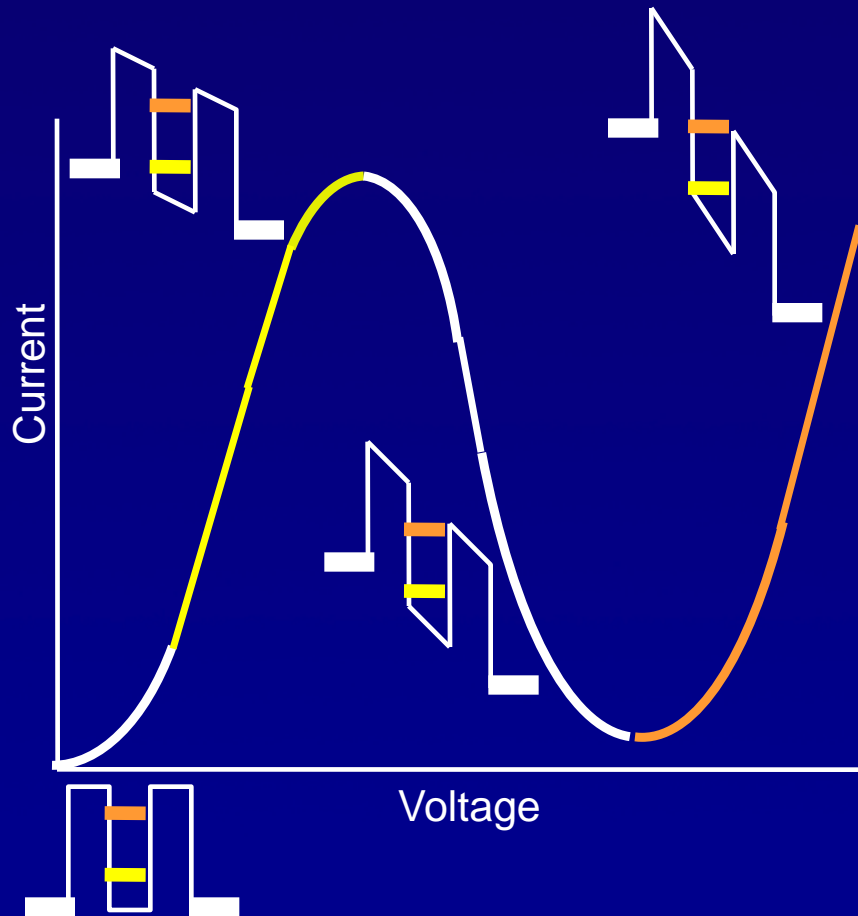
Manhua Leng, Chenjing Fernando, Paul Sotirelis, Carlos Salazar-Lazaro,
Bill McMahon, Daniela Francovicchio, Mukund Swaminathan, Dejan Jovanovic

Experimentalists:

Alan Seabaugh, Ted Moise, Ed Beam, Tom Broekaert,
Paul van der Wagt, Bobby Brar, Y. Chang (all TI), David Chow (HRL)

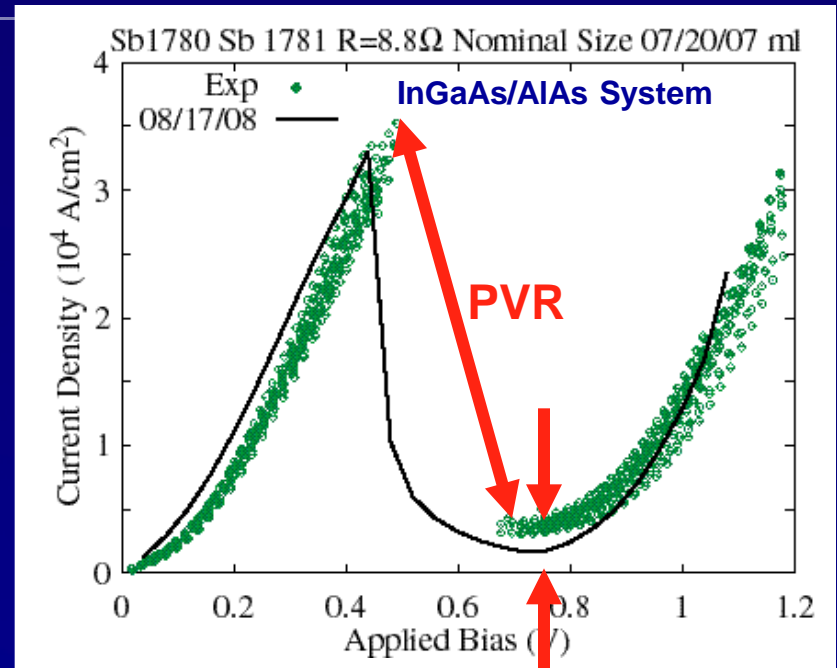
Funding by NRO, ARDA, ONR, NASA, JPL

Basic Operation of a Resonant Tunneling Diode



Conduction band diagrams
for different voltages
and the resulting current flow

NCN



12 different I-V curves: 2 wafers, 3 mesa sizes, 2 bias directions

PVR – Peak-to-Valley-Ratio

1994: Best experiment PVR=80

=> On-Off-Ratio should to be >1,000

1994: What is the valley current physics?

**1997: Can overlay experiment and theory.
What are the key insights?**

Potential:

- THz operation – limited only by tunneling time
- NDR => fast oscillations
- NDR => stable latches, digital logic

Challenges:

- Valley current too high => high “off” state current
- No production-like experiments => repeatability issues
- No generally accepted device modeling theory

⇒ Nanoelectronic Modeling – NEMO

⇒ Software tool that:

- Quantitative modeling
- Predictive design
- Physics-based understanding

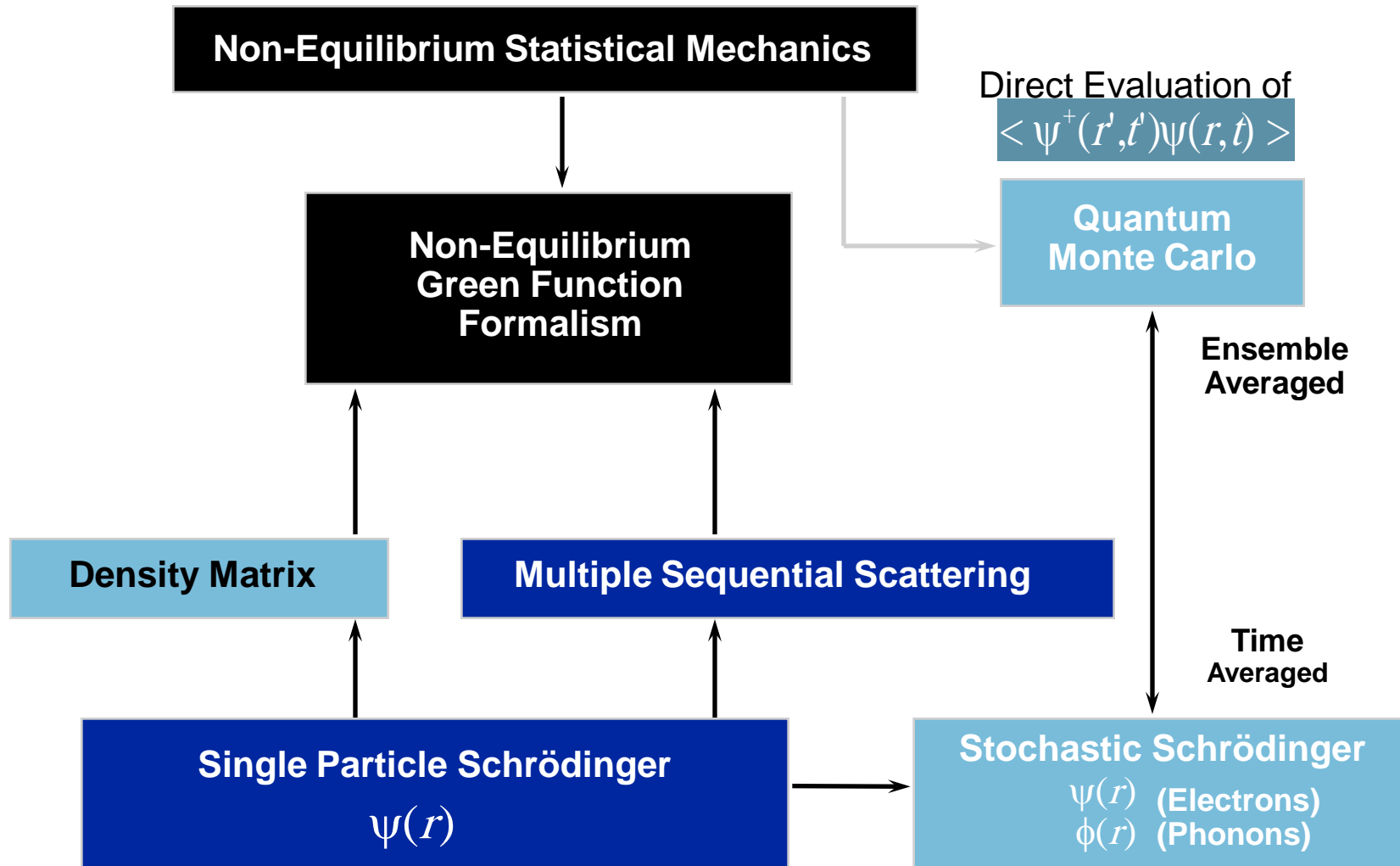
Knowledge / Availability:

- 1-D Poisson Schrödinger
 - » Quantum transmitting boundary conditions (QTBM), flatband (Lent)
 - » Single band, effective mass, no scattering (“everyone”)
 - » Multiple Sequential Scattering (Roblin)
 - » Tight binding, no scattering (Boykin, Ting)
- Density Function
 - » Single band, no scattering, time dependent (Ferry)
- Wigner Function
 - » Single band with empirical scattering (Frensley)
- NEGF
 - » Single band with scattering (Lake, Jauho)
 - » Single band with charge self-consistency (Klimeck)
- **SCATTERING is the source of the valley current**

Limitations:

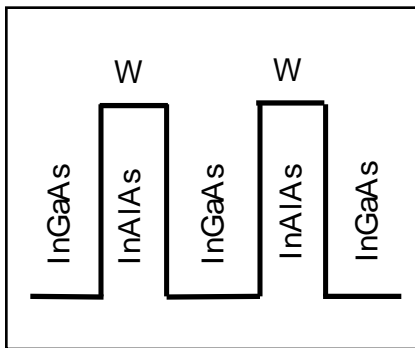
- Tiny device simulation domains – no extended contact regions
- No realistic scattering models
- Computation too expensive for engineering (we can build this in one month)
- No predictive theory, modeling, and simulation

- The non-equilibrium Green function formalism underlies NEMO.
- All of the approaches shown were considered.
- Approaches in light blue were dropped. Approaches in dark blue were incorporated.

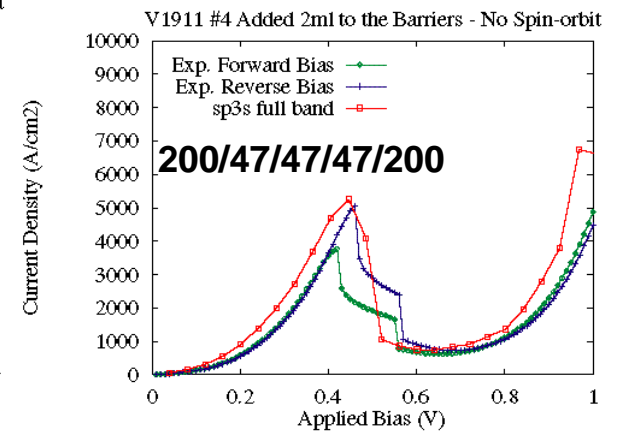
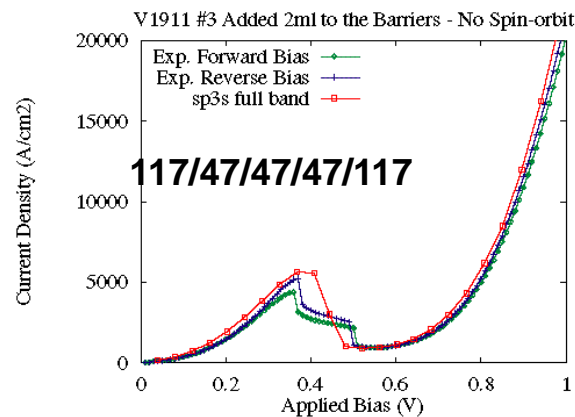
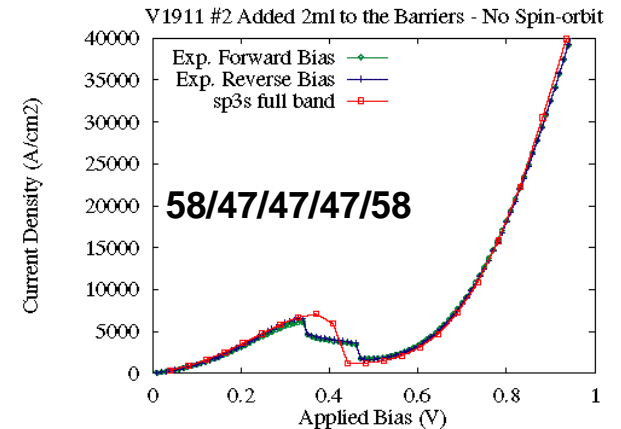
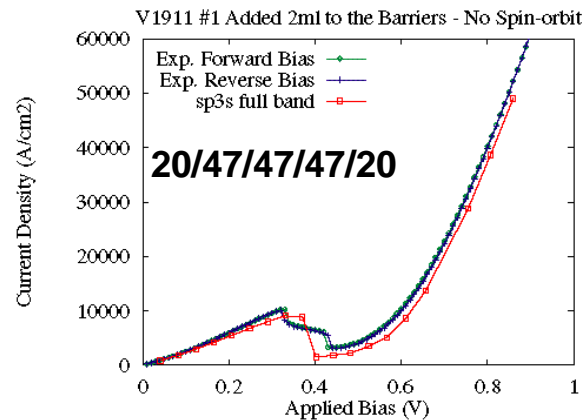


4 Stack RTD with Spacer Variation

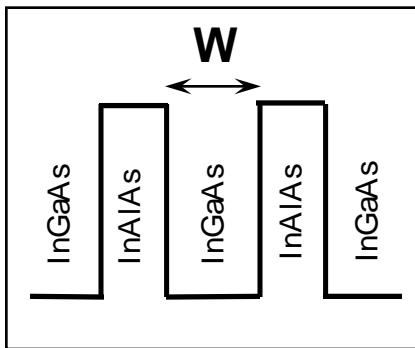
Vary Spacer Length



Four nominally symmetric devices:
20/47/47/47/20 A [1]
58/47/47/47/48 A [2]
117/47/47/47/117 [3]
200/47/47/47/200 [4]



Vary Well Width



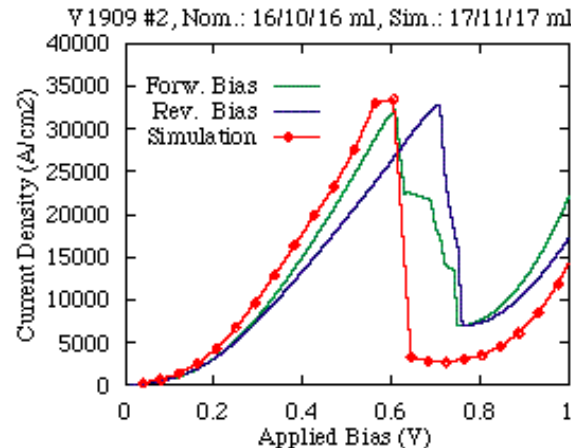
Three nominally symmetric devices:

- 47/29/47 A [1]
- 47/35/47 A [2]
- 47/47/47 A [3]

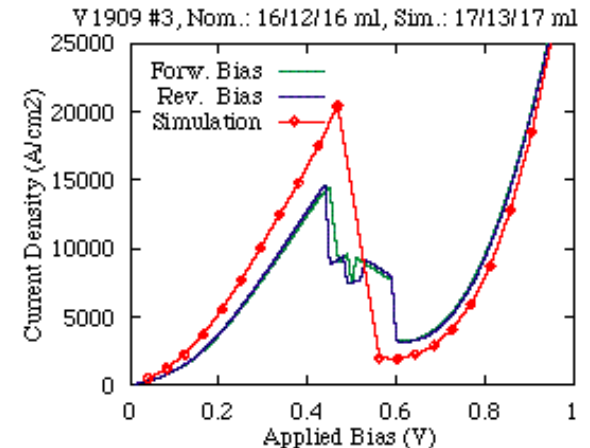
One asymmetric device:

35/47/47 A

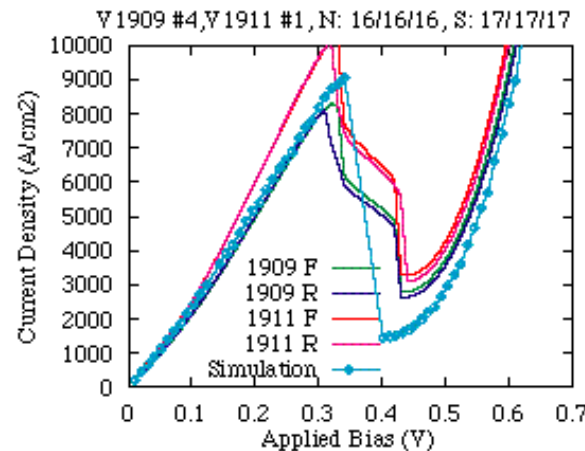
Gerhard Klimeck



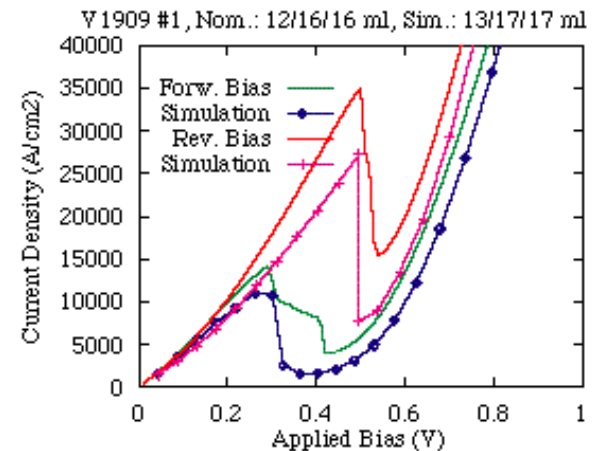
20/47/29/47/20



20/47/35/47/20

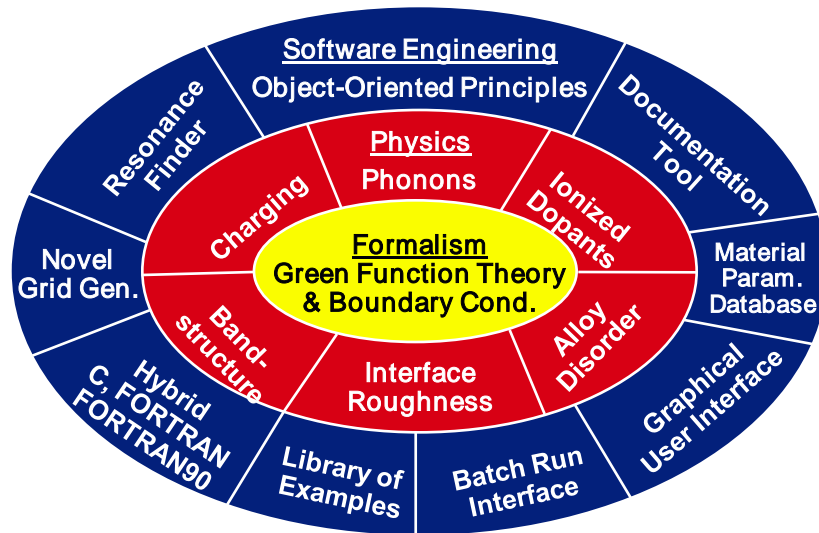
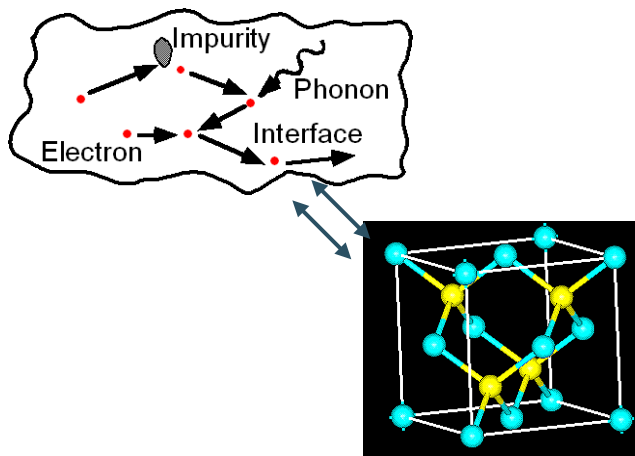


20/47/47/47/20



20/35/47/47/20

- NEMO 1-D was developed under a NSA/NRO contract to Texas Instruments and Raytheon from '93-'98 (>50,000 person hours, 250,000 lines of code).
- NEMO 1-D maintained and NEMO 3-D developed at JPL '98-'03 (>14000 person hours) under NASA, NSA, and ONR funding.
- **NEMO is THE state-of-the-art quantum device design tool.**
 - » First target: transport through resonant tunneling diodes (high speed electronics).
 - » Second target: electronic structure in realistically large nano devices (detectors).
 - » Third target: qbit device simulation.
 - » Ultimate target: Educational tool - heterostructures, bandstructure, transport.
- **Bridges the gap between device engineering and quantum physics.**
- **Based on Non-Equilibrium Green function formalism NEGF - Datta, Lake, Klimeck.**
- **Currently used by limited number of government labs and few Universities.**



Knowledge:

- Scattering inside RTD
 - » Only important at low temperatures
 - » Not important for room temperature, high performance
- Scattering inside extended contacts
 - » Of critical importance at any temperature
- Charge self-consistency
 - » Critical everywhere, contacts and central device
- Bandstructure – atomistic device resolution
 - » Critical for understanding high temperature, high performance devices
- NEGF is the baseline of an industrial strength simulator

Availability:

- An engineering modeling and design tool for 1D heterostructures
- Experimentally verified – **analysis and design**

Even a movie was made!



Currently only available through JPL for government use!

We need public-domain codes as field develops!

The other Nemo has also been found:

