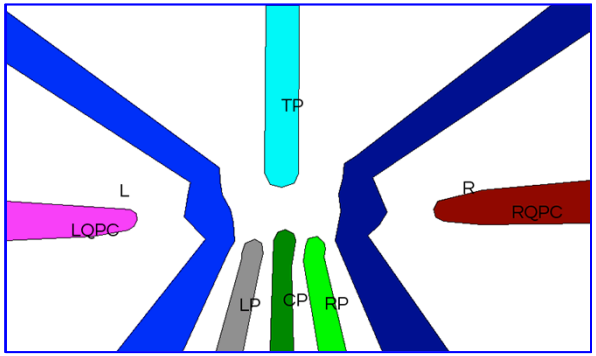
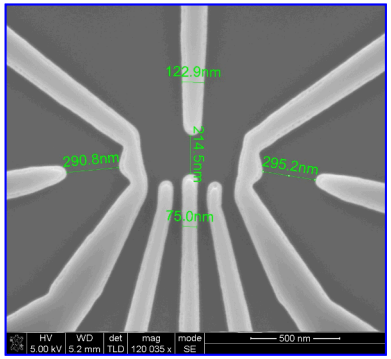
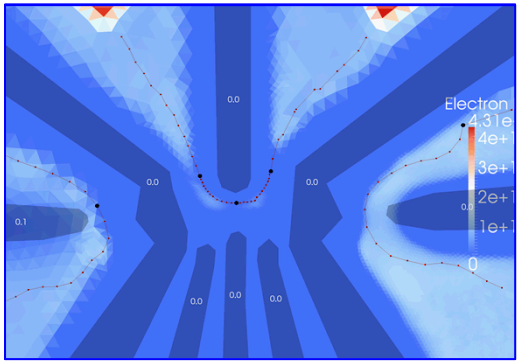
SAND2014-18348PE

Exceptional service in the national interest

Sandia National Laboratories







Modeling Silicon Qubits

Richard P. Muller, Sandia National Laboratories

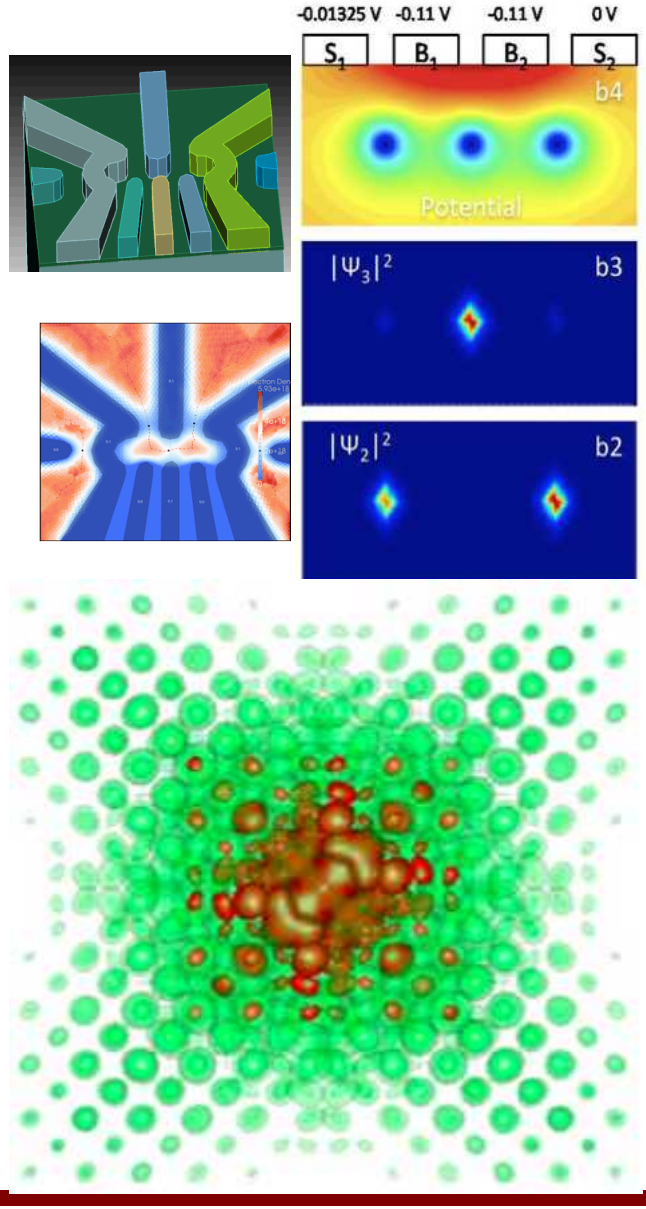
Quantum Materials Workshop, October 2014

U.S. DEPARTMENT OF ENERGY | National Nuclear Security Administration

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

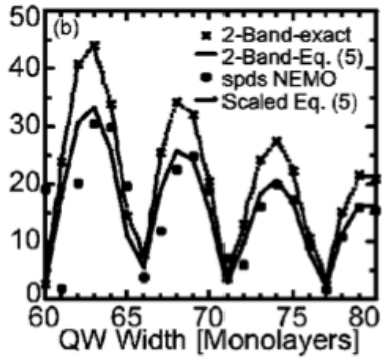
Why is simulating Si qubits hard?

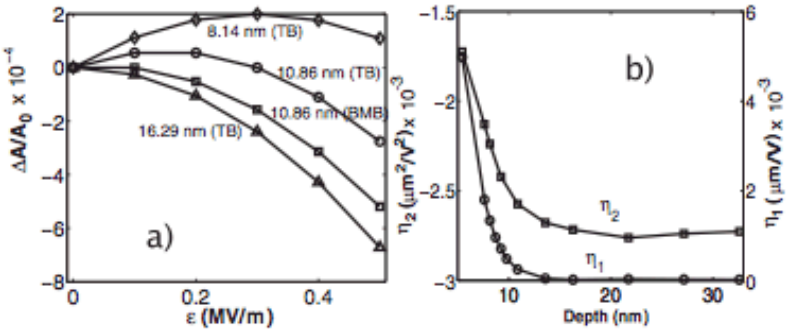
- Size of relevant systems requires huge calculations
- Quantum dots:
  - 100 x 20 x 2 nm ~ 250,000 atoms
  - Need far more atoms for:
    - Oxide
      - And don't understand disorder
    - Gates/ground plane
- Donors
  - Si:P donor 2-4 nm Bohr radius
  - Devices typically at least 60x30x30 nm
    - 1.6 M atoms
- DFT is looking promising:
  - LW Wang (2009): Si:In 64,000 calculation

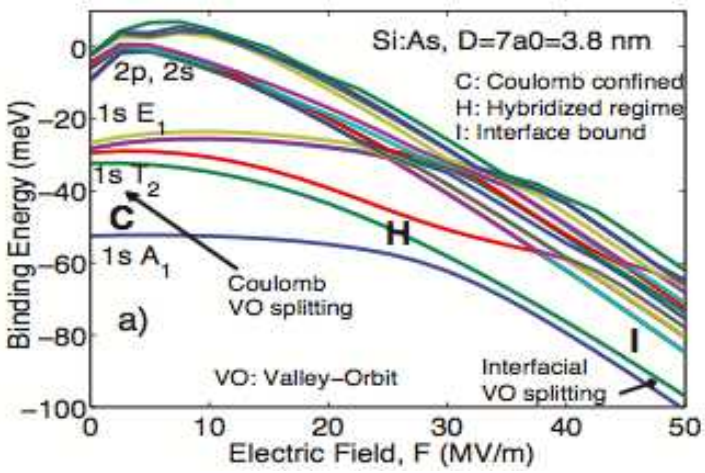


Tight Binding Methods

- Semiempirical parameterization of electronic structure theory
  - Slater/Koster 1954, basic theory
  - Harrison, very compact and transferrable theory for semiconductors
  - Vogl/Hjalmarson/Dow, 1983, sp^3s^* calculations for VB & CB
  - Boykin/Klimeck/Eriksson… 2004, VS as QW width
- NEMO3D, Klimeck:
  - Robust program for high-precision TB calculations for *huge* systems
  - Rahman 2007 Si:P hfine & Stark control
  - Rahman 2009 Si:P donor & interface states

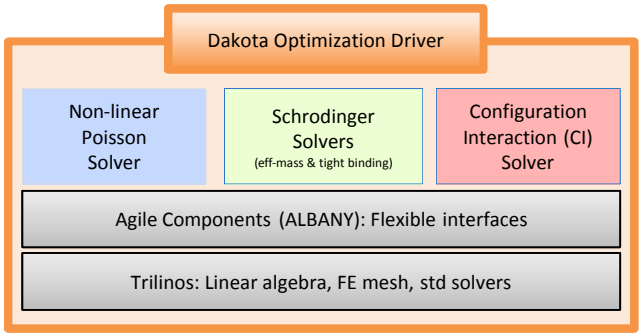


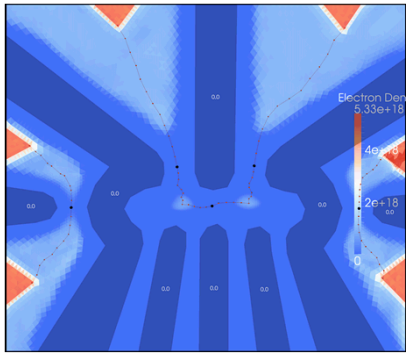


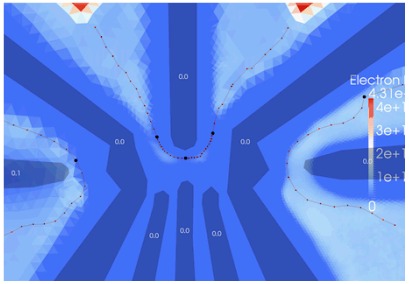


QCAD

- Gao et al. (2013)
- Few-electron, low-T regime is not covered well using existing device modeling tool
- Develop FEM code using SNL/LDRD funding, with some open, parallel tools
- Semiclassical, Schrodinger-Poisson, and Configuration Interaction solvers
- Broad optimization capabilities
- Interface to NEMO3D





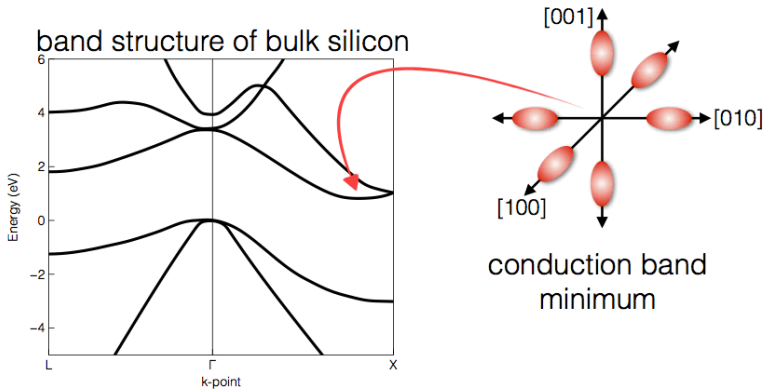


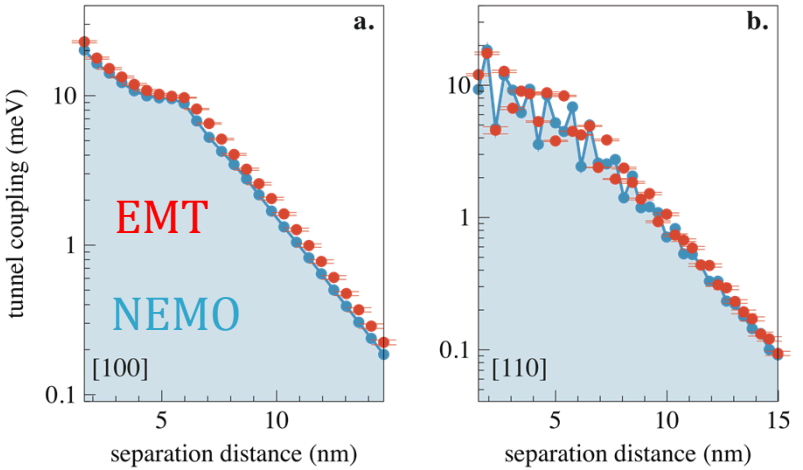
Multivalley EMT

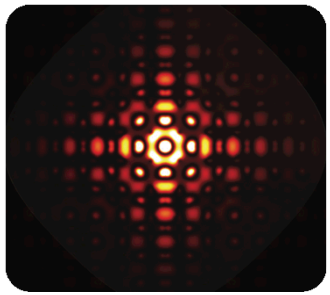
- Seminal work by Kohn/Luttinger, 1955
  - Hfine levels for Group 5 elements

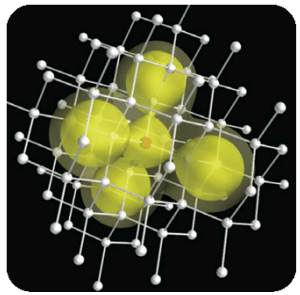
$$F = \sqrt{\frac{a^2 b}{\pi}} \exp\{-\sqrt{a^2\rho^2 + b^2 z^2}\}$$

  - Single-valley, qualitative agreement
- Lot of improvements since then
  - Koiller et al, 2004, Better Bloch functions
  - Ning/Sah, 1971, Central cell correction
- Recent work (Gamble, 2014) combines multivalley EMT, with much more accurate central cell and Bloch functions
  - Near qualitative agreement with tight-binding calculations at a substantially reduced cost, allowing, e.g. millions of scans of tunnel coupling configurations





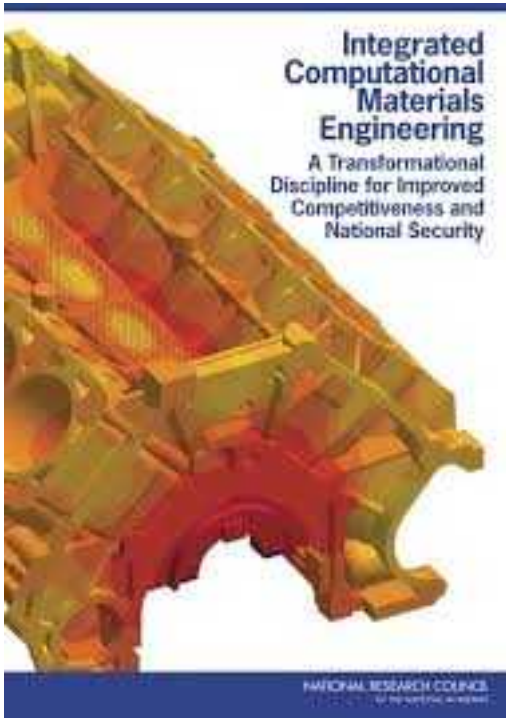




How can we make a big difference?

Sandia National Laboratories

- We need to bring modeling to the point where we can actually do design iterations on a computer rather than in the fab?
- ICME is a good start
  - NRC Report, 2008
  - Appreciates the huge amount of process variation involved in metallurgy and solid mechanics
- We need substantially more sophisticated models for disorder, defects and noise and myriad knobs to tune this with based on empirical data
- We need a huge amount of statistical data so that we can correlate process settings to defect and disorder settings



TMS ICME
MANUFACTURING
DESIGN
MATERIALS

References

- J. Slater and G. Koster, PR **94**, 1498 (1954).
- J. Luttinger and W. Kohn, PR **109**, 1892 (1958).
- T. Ning and C. Sah, PRB **4**, 3468 (1971).
- B. Koiller et al, PRB **70**, 115207 (2004).
- W. Harrison, *Electronic Structure and the Properties of Solids,* 1980.
- P. Vogl, H. Hjalmarson, J. Dow, J Phys Chem Solids, **44,** 365 (1983)
- T.B. Boykin et al., PRB **70**, 12 (2004).
- R. Rahman, et al., PRL (2007).
- J. Allison et al., ICME NRC Report (2008).
- R. Rahman, PRB **80**, 165314 (2009).
- L.-W. Wang, JAP **105**, 123712 (2009).
- X. Gao et al., JAP **114**, 164302 (2013).
- JK Gamble et al., arxiv:1408.2159 (2014)